



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 12:33 PM EDT

PDB ID : 11BE / pdb_000011be
EMDB ID : EMD-6439
Title : HIV-1 Rev Filament
Authors : Eren, E.
Deposited on : 2026-02-15
Resolution : 8.30 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:

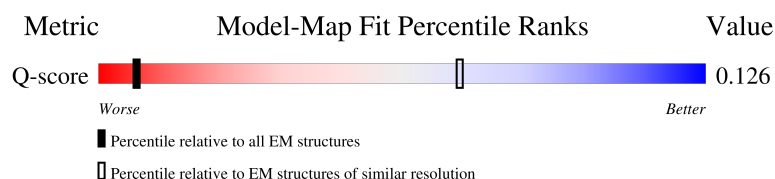
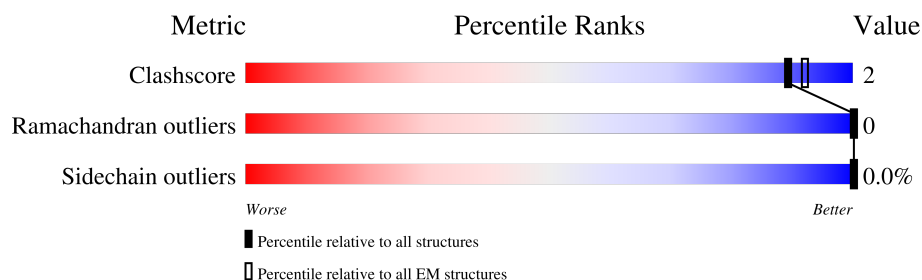
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.30 Å.

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



















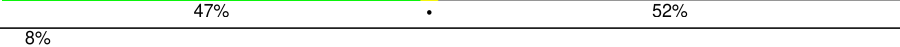
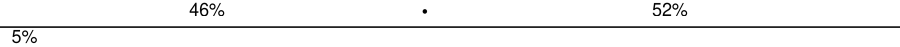
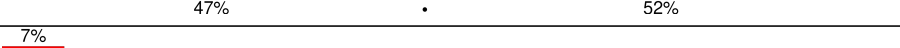
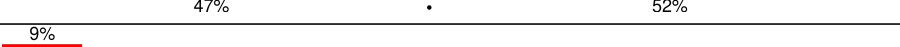

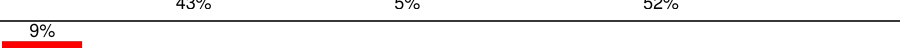

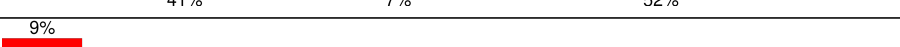
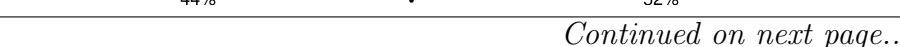
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	280 (7.82 - 8.80)

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	A1	116	<div> <div>9%</div> <div>47%</div> <div>52%</div> </div>
1	A4	116	<div> <div>9%</div> <div>47%</div> <div>52%</div> </div>
1	A5	116	<div> <div>8%</div> <div>47%</div> <div>52%</div> </div>
1	A9	116	<div> <div>8%</div> <div>46%</div> <div>52%</div> </div>

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Mol	Chain	Length	Quality of chain
1	B1	116	
1	B4	116	
1	B5	116	
1	B9	116	
1	C1	116	
1	C5	116	
1	C6	116	
1	C9	116	
1	D1	116	
1	D5	116	
1	D6	116	
1	D9	116	
1	E1	116	
1	E5	116	
1	E6	116	
1	E9	116	
1	F1	116	
1	F5	116	
1	F6	116	
1	F9	116	
1	G1	116	
1	G5	116	
1	G6	116	
1	G9	116	
1	H1	116	

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Mol	Chain	Length	Quality of chain		
1	H5	116	8%	46%	52%
1	H6	116	8%	45%	52%
1	H9	116	8%	44%	52%
1	I1	116	8%	47%	52%
1	I4	116	9%	46%	52%
1	I9	116	8%	46%	52%
1	J1	116	8%	47%	52%
1	J4	116	9%	46%	52%
1	J9	116	8%	47%	52%
1	K1	116	8%	45%	52%
1	K4	116	9%	44%	52%
1	K9	116	9%	45%	52%
1	L1	116	8%	46%	52%
1	L4	116	9%	47%	52%
1	L9	116	5%	47%	52%
1	M1	116	9%	45%	52%
1	M4	116	9%	45%	52%
1	M5	116	10%	46%	52%
1	M9	116	10%	45%	52%
1	N1	116	8%	47%	52%
1	N4	116	8%	47%	52%
1	N5	116	8%	47%	52%
1	N9	116	8%	47%	52%
1	O1	116	8%	47%	52%
1	O4	116	10%	48%	52%




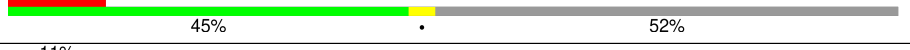




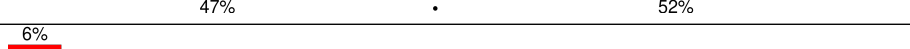
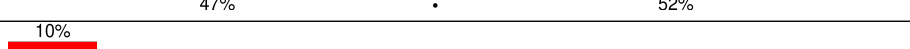
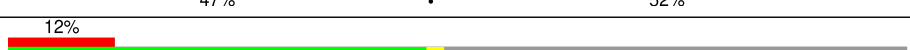

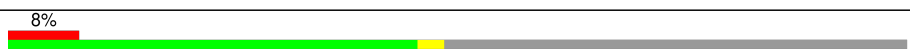
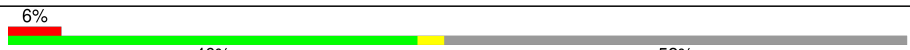
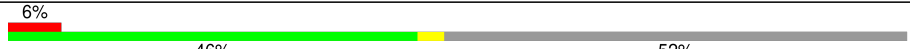










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Mol	Chain	Length	Quality of chain
1	O5	116	
1	O9	116	
1	P1	116	
1	P5	116	
1	P9	116	
1	R1	116	
1	R4	116	
1	R9	116	
1	S1	116	
1	S4	116	
1	S9	116	
1	T1	116	
1	T4	116	
1	T5	116	
1	T9	116	
1	U1	116	
1	U4	116	
1	U5	116	
1	U9	116	
1	V1	116	
1	V5	116	
1	V6	116	
1	V9	116	
1	W1	116	
1	W5	116	

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Mol	Chain	Length	Quality of chain
1	W6	116	
1	W9	116	
1	X1	116	
1	X5	116	
1	X6	116	
1	X9	116	
1	Y1	116	
1	Y5	116	
1	Y6	116	
1	Y9	116	
1	a3	116	
1	a7	116	
1	a8	116	
1	b3	116	
1	b7	116	
1	b8	116	
1	c2	116	
1	c7	116	
1	c8	116	
1	d2	116	
1	d7	116	
1	d8	116	
1	e2	116	
1	e7	116	
1	e8	116	

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Mol	Chain	Length	Quality of chain
1	f2	116	
1	f7	116	
1	f8	116	
1	g2	116	
1	g7	116	
1	g8	116	
1	h2	116	
1	h7	116	
1	h8	116	
1	i3	116	
1	i7	116	
1	j3	116	
1	j7	116	
1	k3	116	
1	k7	116	
1	l3	116	
1	l7	116	
1	m3	116	
1	m7	116	
1	m8	116	
1	n3	116	
1	n7	116	
1	n8	116	
1	o3	116	
1	o7	116	

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Mol	Chain	Length	Quality of chain
1	o8	116	
1	p3	116	
1	p7	116	
1	p8	116	
1	r3	116	
1	r7	116	
1	s3	116	
1	s7	116	
1	t3	116	
1	t7	116	
1	t8	116	
1	u3	116	
1	u7	116	
1	u8	116	
1	v2	116	
1	v7	116	
1	v8	116	
1	w2	116	
1	w7	116	
1	w8	116	
1	x2	116	
1	x7	116	
1	x8	116	
1	y2	116	
1	y7	116	

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Mol	Chain	Length	Quality of chain
1	y8	116	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 76260 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein Rev.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A1	56	Total	C	N	O	0	0
			492	303	112	77		
1	B1	56	Total	C	N	O	0	0
			492	303	112	77		
1	C1	56	Total	C	N	O	0	0
			492	303	112	77		
1	D1	56	Total	C	N	O	0	0
			492	303	112	77		
1	E1	56	Total	C	N	O	0	0
			492	303	112	77		
1	F1	56	Total	C	N	O	0	0
			492	303	112	77		
1	G1	56	Total	C	N	O	0	0
			492	303	112	77		
1	H1	56	Total	C	N	O	0	0
			492	303	112	77		
1	I1	56	Total	C	N	O	0	0
			492	303	112	77		
1	J1	56	Total	C	N	O	0	0
			492	303	112	77		
1	K1	56	Total	C	N	O	0	0
			492	303	112	77		
1	L1	56	Total	C	N	O	0	0
			492	303	112	77		
1	M1	56	Total	C	N	O	0	0
			492	303	112	77		
1	N1	56	Total	C	N	O	0	0
			492	303	112	77		
1	O1	56	Total	C	N	O	0	0
			492	303	112	77		
1	P1	56	Total	C	N	O	0	0
			492	303	112	77		
1	R1	56	Total	C	N	O	0	0
			492	303	112	77		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	S1	56	Total 492	C 303	N 112	O 77	0	0
1	T1	56	Total 492	C 303	N 112	O 77	0	0
1	U1	56	Total 492	C 303	N 112	O 77	0	0
1	V1	56	Total 492	C 303	N 112	O 77	0	0
1	W1	56	Total 492	C 303	N 112	O 77	0	0
1	X1	56	Total 492	C 303	N 112	O 77	0	0
1	Y1	56	Total 492	C 303	N 112	O 77	0	0
1	c2	56	Total 492	C 303	N 112	O 77	0	0
1	d2	56	Total 492	C 303	N 112	O 77	0	0
1	e2	56	Total 492	C 303	N 112	O 77	0	0
1	f2	56	Total 492	C 303	N 112	O 77	0	0
1	g2	56	Total 492	C 303	N 112	O 77	0	0
1	h2	56	Total 492	C 303	N 112	O 77	0	0
1	v2	56	Total 492	C 303	N 112	O 77	0	0
1	w2	56	Total 492	C 303	N 112	O 77	0	0
1	x2	56	Total 492	C 303	N 112	O 77	0	0
1	y2	56	Total 492	C 303	N 112	O 77	0	0
1	a3	56	Total 492	C 303	N 112	O 77	0	0
1	b3	56	Total 492	C 303	N 112	O 77	0	0
1	i3	56	Total 492	C 303	N 112	O 77	0	0
1	j3	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	k3	56	Total 492	C 303	N 112	O 77	0	0
1	l3	56	Total 492	C 303	N 112	O 77	0	0
1	m3	56	Total 492	C 303	N 112	O 77	0	0
1	n3	56	Total 492	C 303	N 112	O 77	0	0
1	o3	56	Total 492	C 303	N 112	O 77	0	0
1	p3	56	Total 492	C 303	N 112	O 77	0	0
1	r3	56	Total 492	C 303	N 112	O 77	0	0
1	s3	56	Total 492	C 303	N 112	O 77	0	0
1	t3	56	Total 492	C 303	N 112	O 77	0	0
1	u3	56	Total 492	C 303	N 112	O 77	0	0
1	A4	56	Total 492	C 303	N 112	O 77	0	0
1	B4	56	Total 492	C 303	N 112	O 77	0	0
1	I4	56	Total 492	C 303	N 112	O 77	0	0
1	J4	56	Total 492	C 303	N 112	O 77	0	0
1	K4	56	Total 492	C 303	N 112	O 77	0	0
1	L4	56	Total 492	C 303	N 112	O 77	0	0
1	M4	56	Total 492	C 303	N 112	O 77	0	0
1	N4	56	Total 492	C 303	N 112	O 77	0	0
1	O4	56	Total 492	C 303	N 112	O 77	0	0
1	R4	56	Total 492	C 303	N 112	O 77	0	0
1	S4	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	T4	56	Total 492	C 303	N 112	O 77	0	0
1	U4	56	Total 492	C 303	N 112	O 77	0	0
1	A5	56	Total 492	C 303	N 112	O 77	0	0
1	B5	56	Total 492	C 303	N 112	O 77	0	0
1	C5	56	Total 492	C 303	N 112	O 77	0	0
1	D5	56	Total 492	C 303	N 112	O 77	0	0
1	E5	56	Total 492	C 303	N 112	O 77	0	0
1	F5	56	Total 492	C 303	N 112	O 77	0	0
1	G5	56	Total 492	C 303	N 112	O 77	0	0
1	H5	56	Total 492	C 303	N 112	O 77	0	0
1	M5	56	Total 492	C 303	N 112	O 77	0	0
1	N5	56	Total 492	C 303	N 112	O 77	0	0
1	O5	56	Total 492	C 303	N 112	O 77	0	0
1	P5	56	Total 492	C 303	N 112	O 77	0	0
1	T5	56	Total 492	C 303	N 112	O 77	0	0
1	U5	56	Total 492	C 303	N 112	O 77	0	0
1	V5	56	Total 492	C 303	N 112	O 77	0	0
1	W5	56	Total 492	C 303	N 112	O 77	0	0
1	X5	56	Total 492	C 303	N 112	O 77	0	0
1	Y5	56	Total 492	C 303	N 112	O 77	0	0
1	C6	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	D6	56	Total 492	C 303	N 112	O 77	0	0
1	E6	56	Total 492	C 303	N 112	O 77	0	0
1	F6	56	Total 492	C 303	N 112	O 77	0	0
1	G6	56	Total 492	C 303	N 112	O 77	0	0
1	H6	56	Total 492	C 303	N 112	O 77	0	0
1	V6	56	Total 492	C 303	N 112	O 77	0	0
1	W6	56	Total 492	C 303	N 112	O 77	0	0
1	X6	56	Total 492	C 303	N 112	O 77	0	0
1	Y6	56	Total 492	C 303	N 112	O 77	0	0
1	a7	56	Total 492	C 303	N 112	O 77	0	0
1	b7	56	Total 492	C 303	N 112	O 77	0	0
1	c7	56	Total 492	C 303	N 112	O 77	0	0
1	d7	56	Total 492	C 303	N 112	O 77	0	0
1	e7	56	Total 492	C 303	N 112	O 77	0	0
1	f7	56	Total 492	C 303	N 112	O 77	0	0
1	g7	56	Total 492	C 303	N 112	O 77	0	0
1	h7	56	Total 492	C 303	N 112	O 77	0	0
1	i7	56	Total 492	C 303	N 112	O 77	0	0
1	j7	56	Total 492	C 303	N 112	O 77	0	0
1	k7	56	Total 492	C 303	N 112	O 77	0	0
1	l7	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	m7	56	Total 492	C 303	N 112	O 77	0	0
1	n7	56	Total 492	C 303	N 112	O 77	0	0
1	o7	56	Total 492	C 303	N 112	O 77	0	0
1	p7	56	Total 492	C 303	N 112	O 77	0	0
1	r7	56	Total 492	C 303	N 112	O 77	0	0
1	s7	56	Total 492	C 303	N 112	O 77	0	0
1	t7	56	Total 492	C 303	N 112	O 77	0	0
1	u7	56	Total 492	C 303	N 112	O 77	0	0
1	v7	56	Total 492	C 303	N 112	O 77	0	0
1	w7	56	Total 492	C 303	N 112	O 77	0	0
1	x7	56	Total 492	C 303	N 112	O 77	0	0
1	y7	56	Total 492	C 303	N 112	O 77	0	0
1	a8	56	Total 492	C 303	N 112	O 77	0	0
1	b8	56	Total 492	C 303	N 112	O 77	0	0
1	c8	56	Total 492	C 303	N 112	O 77	0	0
1	d8	56	Total 492	C 303	N 112	O 77	0	0
1	e8	56	Total 492	C 303	N 112	O 77	0	0
1	f8	56	Total 492	C 303	N 112	O 77	0	0
1	g8	56	Total 492	C 303	N 112	O 77	0	0
1	h8	56	Total 492	C 303	N 112	O 77	0	0
1	m8	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	n8	56	Total 492	C 303	N 112	O 77	0	0
1	o8	56	Total 492	C 303	N 112	O 77	0	0
1	p8	56	Total 492	C 303	N 112	O 77	0	0
1	t8	56	Total 492	C 303	N 112	O 77	0	0
1	u8	56	Total 492	C 303	N 112	O 77	0	0
1	v8	56	Total 492	C 303	N 112	O 77	0	0
1	w8	56	Total 492	C 303	N 112	O 77	0	0
1	x8	56	Total 492	C 303	N 112	O 77	0	0
1	y8	56	Total 492	C 303	N 112	O 77	0	0
1	A9	56	Total 492	C 303	N 112	O 77	0	0
1	B9	56	Total 492	C 303	N 112	O 77	0	0
1	C9	56	Total 492	C 303	N 112	O 77	0	0
1	D9	56	Total 492	C 303	N 112	O 77	0	0
1	E9	56	Total 492	C 303	N 112	O 77	0	0
1	F9	56	Total 492	C 303	N 112	O 77	0	0
1	G9	56	Total 492	C 303	N 112	O 77	0	0
1	H9	56	Total 492	C 303	N 112	O 77	0	0
1	I9	56	Total 492	C 303	N 112	O 77	0	0
1	J9	56	Total 492	C 303	N 112	O 77	0	0
1	K9	56	Total 492	C 303	N 112	O 77	0	0
1	L9	56	Total 492	C 303	N 112	O 77	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	M9	56	Total 492	C 303	N 112	O 77	0	0
1	N9	56	Total 492	C 303	N 112	O 77	0	0
1	O9	56	Total 492	C 303	N 112	O 77	0	0
1	P9	56	Total 492	C 303	N 112	O 77	0	0
1	R9	56	Total 492	C 303	N 112	O 77	0	0
1	S9	56	Total 492	C 303	N 112	O 77	0	0
1	T9	56	Total 492	C 303	N 112	O 77	0	0
1	U9	56	Total 492	C 303	N 112	O 77	0	0
1	V9	56	Total 492	C 303	N 112	O 77	0	0
1	W9	56	Total 492	C 303	N 112	O 77	0	0
1	X9	56	Total 492	C 303	N 112	O 77	0	0
1	Y9	56	Total 492	C 303	N 112	O 77	0	0

There are 620 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	15	THR	ALA	conflict	UNP Q76PP8
A1	49	ARG	GLN	conflict	UNP Q76PP8
A1	57	ARG	GLU	conflict	UNP Q76PP8
A1	109	VAL	ILE	conflict	UNP Q76PP8
B1	15	THR	ALA	conflict	UNP Q76PP8
B1	49	ARG	GLN	conflict	UNP Q76PP8
B1	57	ARG	GLU	conflict	UNP Q76PP8
B1	109	VAL	ILE	conflict	UNP Q76PP8
C1	15	THR	ALA	conflict	UNP Q76PP8
C1	49	ARG	GLN	conflict	UNP Q76PP8
C1	57	ARG	GLU	conflict	UNP Q76PP8
C1	109	VAL	ILE	conflict	UNP Q76PP8
D1	15	THR	ALA	conflict	UNP Q76PP8
D1	49	ARG	GLN	conflict	UNP Q76PP8
D1	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
D1	109	VAL	ILE	conflict	UNP Q76PP8
E1	15	THR	ALA	conflict	UNP Q76PP8
E1	49	ARG	GLN	conflict	UNP Q76PP8
E1	57	ARG	GLU	conflict	UNP Q76PP8
E1	109	VAL	ILE	conflict	UNP Q76PP8
F1	15	THR	ALA	conflict	UNP Q76PP8
F1	49	ARG	GLN	conflict	UNP Q76PP8
F1	57	ARG	GLU	conflict	UNP Q76PP8
F1	109	VAL	ILE	conflict	UNP Q76PP8
G1	15	THR	ALA	conflict	UNP Q76PP8
G1	49	ARG	GLN	conflict	UNP Q76PP8
G1	57	ARG	GLU	conflict	UNP Q76PP8
G1	109	VAL	ILE	conflict	UNP Q76PP8
H1	15	THR	ALA	conflict	UNP Q76PP8
H1	49	ARG	GLN	conflict	UNP Q76PP8
H1	57	ARG	GLU	conflict	UNP Q76PP8
H1	109	VAL	ILE	conflict	UNP Q76PP8
I1	15	THR	ALA	conflict	UNP Q76PP8
I1	49	ARG	GLN	conflict	UNP Q76PP8
I1	57	ARG	GLU	conflict	UNP Q76PP8
I1	109	VAL	ILE	conflict	UNP Q76PP8
J1	15	THR	ALA	conflict	UNP Q76PP8
J1	49	ARG	GLN	conflict	UNP Q76PP8
J1	57	ARG	GLU	conflict	UNP Q76PP8
J1	109	VAL	ILE	conflict	UNP Q76PP8
K1	15	THR	ALA	conflict	UNP Q76PP8
K1	49	ARG	GLN	conflict	UNP Q76PP8
K1	57	ARG	GLU	conflict	UNP Q76PP8
K1	109	VAL	ILE	conflict	UNP Q76PP8
L1	15	THR	ALA	conflict	UNP Q76PP8
L1	49	ARG	GLN	conflict	UNP Q76PP8
L1	57	ARG	GLU	conflict	UNP Q76PP8
L1	109	VAL	ILE	conflict	UNP Q76PP8
M1	15	THR	ALA	conflict	UNP Q76PP8
M1	49	ARG	GLN	conflict	UNP Q76PP8
M1	57	ARG	GLU	conflict	UNP Q76PP8
M1	109	VAL	ILE	conflict	UNP Q76PP8
N1	15	THR	ALA	conflict	UNP Q76PP8
N1	49	ARG	GLN	conflict	UNP Q76PP8
N1	57	ARG	GLU	conflict	UNP Q76PP8
N1	109	VAL	ILE	conflict	UNP Q76PP8
O1	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
O1	49	ARG	GLN	conflict	UNP Q76PP8
O1	57	ARG	GLU	conflict	UNP Q76PP8
O1	109	VAL	ILE	conflict	UNP Q76PP8
P1	15	THR	ALA	conflict	UNP Q76PP8
P1	49	ARG	GLN	conflict	UNP Q76PP8
P1	57	ARG	GLU	conflict	UNP Q76PP8
P1	109	VAL	ILE	conflict	UNP Q76PP8
R1	15	THR	ALA	conflict	UNP Q76PP8
R1	49	ARG	GLN	conflict	UNP Q76PP8
R1	57	ARG	GLU	conflict	UNP Q76PP8
R1	109	VAL	ILE	conflict	UNP Q76PP8
S1	15	THR	ALA	conflict	UNP Q76PP8
S1	49	ARG	GLN	conflict	UNP Q76PP8
S1	57	ARG	GLU	conflict	UNP Q76PP8
S1	109	VAL	ILE	conflict	UNP Q76PP8
T1	15	THR	ALA	conflict	UNP Q76PP8
T1	49	ARG	GLN	conflict	UNP Q76PP8
T1	57	ARG	GLU	conflict	UNP Q76PP8
T1	109	VAL	ILE	conflict	UNP Q76PP8
U1	15	THR	ALA	conflict	UNP Q76PP8
U1	49	ARG	GLN	conflict	UNP Q76PP8
U1	57	ARG	GLU	conflict	UNP Q76PP8
U1	109	VAL	ILE	conflict	UNP Q76PP8
V1	15	THR	ALA	conflict	UNP Q76PP8
V1	49	ARG	GLN	conflict	UNP Q76PP8
V1	57	ARG	GLU	conflict	UNP Q76PP8
V1	109	VAL	ILE	conflict	UNP Q76PP8
W1	15	THR	ALA	conflict	UNP Q76PP8
W1	49	ARG	GLN	conflict	UNP Q76PP8
W1	57	ARG	GLU	conflict	UNP Q76PP8
W1	109	VAL	ILE	conflict	UNP Q76PP8
X1	15	THR	ALA	conflict	UNP Q76PP8
X1	49	ARG	GLN	conflict	UNP Q76PP8
X1	57	ARG	GLU	conflict	UNP Q76PP8
X1	109	VAL	ILE	conflict	UNP Q76PP8
Y1	15	THR	ALA	conflict	UNP Q76PP8
Y1	49	ARG	GLN	conflict	UNP Q76PP8
Y1	57	ARG	GLU	conflict	UNP Q76PP8
Y1	109	VAL	ILE	conflict	UNP Q76PP8
c2	15	THR	ALA	conflict	UNP Q76PP8
c2	49	ARG	GLN	conflict	UNP Q76PP8
c2	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
c2	109	VAL	ILE	conflict	UNP Q76PP8
d2	15	THR	ALA	conflict	UNP Q76PP8
d2	49	ARG	GLN	conflict	UNP Q76PP8
d2	57	ARG	GLU	conflict	UNP Q76PP8
d2	109	VAL	ILE	conflict	UNP Q76PP8
e2	15	THR	ALA	conflict	UNP Q76PP8
e2	49	ARG	GLN	conflict	UNP Q76PP8
e2	57	ARG	GLU	conflict	UNP Q76PP8
e2	109	VAL	ILE	conflict	UNP Q76PP8
f2	15	THR	ALA	conflict	UNP Q76PP8
f2	49	ARG	GLN	conflict	UNP Q76PP8
f2	57	ARG	GLU	conflict	UNP Q76PP8
f2	109	VAL	ILE	conflict	UNP Q76PP8
g2	15	THR	ALA	conflict	UNP Q76PP8
g2	49	ARG	GLN	conflict	UNP Q76PP8
g2	57	ARG	GLU	conflict	UNP Q76PP8
g2	109	VAL	ILE	conflict	UNP Q76PP8
h2	15	THR	ALA	conflict	UNP Q76PP8
h2	49	ARG	GLN	conflict	UNP Q76PP8
h2	57	ARG	GLU	conflict	UNP Q76PP8
h2	109	VAL	ILE	conflict	UNP Q76PP8
v2	15	THR	ALA	conflict	UNP Q76PP8
v2	49	ARG	GLN	conflict	UNP Q76PP8
v2	57	ARG	GLU	conflict	UNP Q76PP8
v2	109	VAL	ILE	conflict	UNP Q76PP8
w2	15	THR	ALA	conflict	UNP Q76PP8
w2	49	ARG	GLN	conflict	UNP Q76PP8
w2	57	ARG	GLU	conflict	UNP Q76PP8
w2	109	VAL	ILE	conflict	UNP Q76PP8
x2	15	THR	ALA	conflict	UNP Q76PP8
x2	49	ARG	GLN	conflict	UNP Q76PP8
x2	57	ARG	GLU	conflict	UNP Q76PP8
x2	109	VAL	ILE	conflict	UNP Q76PP8
y2	15	THR	ALA	conflict	UNP Q76PP8
y2	49	ARG	GLN	conflict	UNP Q76PP8
y2	57	ARG	GLU	conflict	UNP Q76PP8
y2	109	VAL	ILE	conflict	UNP Q76PP8
a3	15	THR	ALA	conflict	UNP Q76PP8
a3	49	ARG	GLN	conflict	UNP Q76PP8
a3	57	ARG	GLU	conflict	UNP Q76PP8
a3	109	VAL	ILE	conflict	UNP Q76PP8
b3	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
b3	49	ARG	GLN	conflict	UNP Q76PP8
b3	57	ARG	GLU	conflict	UNP Q76PP8
b3	109	VAL	ILE	conflict	UNP Q76PP8
i3	15	THR	ALA	conflict	UNP Q76PP8
i3	49	ARG	GLN	conflict	UNP Q76PP8
i3	57	ARG	GLU	conflict	UNP Q76PP8
i3	109	VAL	ILE	conflict	UNP Q76PP8
j3	15	THR	ALA	conflict	UNP Q76PP8
j3	49	ARG	GLN	conflict	UNP Q76PP8
j3	57	ARG	GLU	conflict	UNP Q76PP8
j3	109	VAL	ILE	conflict	UNP Q76PP8
k3	15	THR	ALA	conflict	UNP Q76PP8
k3	49	ARG	GLN	conflict	UNP Q76PP8
k3	57	ARG	GLU	conflict	UNP Q76PP8
k3	109	VAL	ILE	conflict	UNP Q76PP8
l3	15	THR	ALA	conflict	UNP Q76PP8
l3	49	ARG	GLN	conflict	UNP Q76PP8
l3	57	ARG	GLU	conflict	UNP Q76PP8
l3	109	VAL	ILE	conflict	UNP Q76PP8
m3	15	THR	ALA	conflict	UNP Q76PP8
m3	49	ARG	GLN	conflict	UNP Q76PP8
m3	57	ARG	GLU	conflict	UNP Q76PP8
m3	109	VAL	ILE	conflict	UNP Q76PP8
n3	15	THR	ALA	conflict	UNP Q76PP8
n3	49	ARG	GLN	conflict	UNP Q76PP8
n3	57	ARG	GLU	conflict	UNP Q76PP8
n3	109	VAL	ILE	conflict	UNP Q76PP8
o3	15	THR	ALA	conflict	UNP Q76PP8
o3	49	ARG	GLN	conflict	UNP Q76PP8
o3	57	ARG	GLU	conflict	UNP Q76PP8
o3	109	VAL	ILE	conflict	UNP Q76PP8
p3	15	THR	ALA	conflict	UNP Q76PP8
p3	49	ARG	GLN	conflict	UNP Q76PP8
p3	57	ARG	GLU	conflict	UNP Q76PP8
p3	109	VAL	ILE	conflict	UNP Q76PP8
r3	15	THR	ALA	conflict	UNP Q76PP8
r3	49	ARG	GLN	conflict	UNP Q76PP8
r3	57	ARG	GLU	conflict	UNP Q76PP8
r3	109	VAL	ILE	conflict	UNP Q76PP8
s3	15	THR	ALA	conflict	UNP Q76PP8
s3	49	ARG	GLN	conflict	UNP Q76PP8
s3	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
s3	109	VAL	ILE	conflict	UNP Q76PP8
t3	15	THR	ALA	conflict	UNP Q76PP8
t3	49	ARG	GLN	conflict	UNP Q76PP8
t3	57	ARG	GLU	conflict	UNP Q76PP8
t3	109	VAL	ILE	conflict	UNP Q76PP8
u3	15	THR	ALA	conflict	UNP Q76PP8
u3	49	ARG	GLN	conflict	UNP Q76PP8
u3	57	ARG	GLU	conflict	UNP Q76PP8
u3	109	VAL	ILE	conflict	UNP Q76PP8
A4	15	THR	ALA	conflict	UNP Q76PP8
A4	49	ARG	GLN	conflict	UNP Q76PP8
A4	57	ARG	GLU	conflict	UNP Q76PP8
A4	109	VAL	ILE	conflict	UNP Q76PP8
B4	15	THR	ALA	conflict	UNP Q76PP8
B4	49	ARG	GLN	conflict	UNP Q76PP8
B4	57	ARG	GLU	conflict	UNP Q76PP8
B4	109	VAL	ILE	conflict	UNP Q76PP8
I4	15	THR	ALA	conflict	UNP Q76PP8
I4	49	ARG	GLN	conflict	UNP Q76PP8
I4	57	ARG	GLU	conflict	UNP Q76PP8
I4	109	VAL	ILE	conflict	UNP Q76PP8
J4	15	THR	ALA	conflict	UNP Q76PP8
J4	49	ARG	GLN	conflict	UNP Q76PP8
J4	57	ARG	GLU	conflict	UNP Q76PP8
J4	109	VAL	ILE	conflict	UNP Q76PP8
K4	15	THR	ALA	conflict	UNP Q76PP8
K4	49	ARG	GLN	conflict	UNP Q76PP8
K4	57	ARG	GLU	conflict	UNP Q76PP8
K4	109	VAL	ILE	conflict	UNP Q76PP8
L4	15	THR	ALA	conflict	UNP Q76PP8
L4	49	ARG	GLN	conflict	UNP Q76PP8
L4	57	ARG	GLU	conflict	UNP Q76PP8
L4	109	VAL	ILE	conflict	UNP Q76PP8
M4	15	THR	ALA	conflict	UNP Q76PP8
M4	49	ARG	GLN	conflict	UNP Q76PP8
M4	57	ARG	GLU	conflict	UNP Q76PP8
M4	109	VAL	ILE	conflict	UNP Q76PP8
N4	15	THR	ALA	conflict	UNP Q76PP8
N4	49	ARG	GLN	conflict	UNP Q76PP8
N4	57	ARG	GLU	conflict	UNP Q76PP8
N4	109	VAL	ILE	conflict	UNP Q76PP8
O4	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
O4	49	ARG	GLN	conflict	UNP Q76PP8
O4	57	ARG	GLU	conflict	UNP Q76PP8
O4	109	VAL	ILE	conflict	UNP Q76PP8
R4	15	THR	ALA	conflict	UNP Q76PP8
R4	49	ARG	GLN	conflict	UNP Q76PP8
R4	57	ARG	GLU	conflict	UNP Q76PP8
R4	109	VAL	ILE	conflict	UNP Q76PP8
S4	15	THR	ALA	conflict	UNP Q76PP8
S4	49	ARG	GLN	conflict	UNP Q76PP8
S4	57	ARG	GLU	conflict	UNP Q76PP8
S4	109	VAL	ILE	conflict	UNP Q76PP8
T4	15	THR	ALA	conflict	UNP Q76PP8
T4	49	ARG	GLN	conflict	UNP Q76PP8
T4	57	ARG	GLU	conflict	UNP Q76PP8
T4	109	VAL	ILE	conflict	UNP Q76PP8
U4	15	THR	ALA	conflict	UNP Q76PP8
U4	49	ARG	GLN	conflict	UNP Q76PP8
U4	57	ARG	GLU	conflict	UNP Q76PP8
U4	109	VAL	ILE	conflict	UNP Q76PP8
A5	15	THR	ALA	conflict	UNP Q76PP8
A5	49	ARG	GLN	conflict	UNP Q76PP8
A5	57	ARG	GLU	conflict	UNP Q76PP8
A5	109	VAL	ILE	conflict	UNP Q76PP8
B5	15	THR	ALA	conflict	UNP Q76PP8
B5	49	ARG	GLN	conflict	UNP Q76PP8
B5	57	ARG	GLU	conflict	UNP Q76PP8
B5	109	VAL	ILE	conflict	UNP Q76PP8
C5	15	THR	ALA	conflict	UNP Q76PP8
C5	49	ARG	GLN	conflict	UNP Q76PP8
C5	57	ARG	GLU	conflict	UNP Q76PP8
C5	109	VAL	ILE	conflict	UNP Q76PP8
D5	15	THR	ALA	conflict	UNP Q76PP8
D5	49	ARG	GLN	conflict	UNP Q76PP8
D5	57	ARG	GLU	conflict	UNP Q76PP8
D5	109	VAL	ILE	conflict	UNP Q76PP8
E5	15	THR	ALA	conflict	UNP Q76PP8
E5	49	ARG	GLN	conflict	UNP Q76PP8
E5	57	ARG	GLU	conflict	UNP Q76PP8
E5	109	VAL	ILE	conflict	UNP Q76PP8
F5	15	THR	ALA	conflict	UNP Q76PP8
F5	49	ARG	GLN	conflict	UNP Q76PP8
F5	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
F5	109	VAL	ILE	conflict	UNP Q76PP8
G5	15	THR	ALA	conflict	UNP Q76PP8
G5	49	ARG	GLN	conflict	UNP Q76PP8
G5	57	ARG	GLU	conflict	UNP Q76PP8
G5	109	VAL	ILE	conflict	UNP Q76PP8
H5	15	THR	ALA	conflict	UNP Q76PP8
H5	49	ARG	GLN	conflict	UNP Q76PP8
H5	57	ARG	GLU	conflict	UNP Q76PP8
H5	109	VAL	ILE	conflict	UNP Q76PP8
M5	15	THR	ALA	conflict	UNP Q76PP8
M5	49	ARG	GLN	conflict	UNP Q76PP8
M5	57	ARG	GLU	conflict	UNP Q76PP8
M5	109	VAL	ILE	conflict	UNP Q76PP8
N5	15	THR	ALA	conflict	UNP Q76PP8
N5	49	ARG	GLN	conflict	UNP Q76PP8
N5	57	ARG	GLU	conflict	UNP Q76PP8
N5	109	VAL	ILE	conflict	UNP Q76PP8
O5	15	THR	ALA	conflict	UNP Q76PP8
O5	49	ARG	GLN	conflict	UNP Q76PP8
O5	57	ARG	GLU	conflict	UNP Q76PP8
O5	109	VAL	ILE	conflict	UNP Q76PP8
P5	15	THR	ALA	conflict	UNP Q76PP8
P5	49	ARG	GLN	conflict	UNP Q76PP8
P5	57	ARG	GLU	conflict	UNP Q76PP8
P5	109	VAL	ILE	conflict	UNP Q76PP8
T5	15	THR	ALA	conflict	UNP Q76PP8
T5	49	ARG	GLN	conflict	UNP Q76PP8
T5	57	ARG	GLU	conflict	UNP Q76PP8
T5	109	VAL	ILE	conflict	UNP Q76PP8
U5	15	THR	ALA	conflict	UNP Q76PP8
U5	49	ARG	GLN	conflict	UNP Q76PP8
U5	57	ARG	GLU	conflict	UNP Q76PP8
U5	109	VAL	ILE	conflict	UNP Q76PP8
V5	15	THR	ALA	conflict	UNP Q76PP8
V5	49	ARG	GLN	conflict	UNP Q76PP8
V5	57	ARG	GLU	conflict	UNP Q76PP8
V5	109	VAL	ILE	conflict	UNP Q76PP8
W5	15	THR	ALA	conflict	UNP Q76PP8
W5	49	ARG	GLN	conflict	UNP Q76PP8
W5	57	ARG	GLU	conflict	UNP Q76PP8
W5	109	VAL	ILE	conflict	UNP Q76PP8
X5	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
X5	49	ARG	GLN	conflict	UNP Q76PP8
X5	57	ARG	GLU	conflict	UNP Q76PP8
X5	109	VAL	ILE	conflict	UNP Q76PP8
Y5	15	THR	ALA	conflict	UNP Q76PP8
Y5	49	ARG	GLN	conflict	UNP Q76PP8
Y5	57	ARG	GLU	conflict	UNP Q76PP8
Y5	109	VAL	ILE	conflict	UNP Q76PP8
C6	15	THR	ALA	conflict	UNP Q76PP8
C6	49	ARG	GLN	conflict	UNP Q76PP8
C6	57	ARG	GLU	conflict	UNP Q76PP8
C6	109	VAL	ILE	conflict	UNP Q76PP8
D6	15	THR	ALA	conflict	UNP Q76PP8
D6	49	ARG	GLN	conflict	UNP Q76PP8
D6	57	ARG	GLU	conflict	UNP Q76PP8
D6	109	VAL	ILE	conflict	UNP Q76PP8
E6	15	THR	ALA	conflict	UNP Q76PP8
E6	49	ARG	GLN	conflict	UNP Q76PP8
E6	57	ARG	GLU	conflict	UNP Q76PP8
E6	109	VAL	ILE	conflict	UNP Q76PP8
F6	15	THR	ALA	conflict	UNP Q76PP8
F6	49	ARG	GLN	conflict	UNP Q76PP8
F6	57	ARG	GLU	conflict	UNP Q76PP8
F6	109	VAL	ILE	conflict	UNP Q76PP8
G6	15	THR	ALA	conflict	UNP Q76PP8
G6	49	ARG	GLN	conflict	UNP Q76PP8
G6	57	ARG	GLU	conflict	UNP Q76PP8
G6	109	VAL	ILE	conflict	UNP Q76PP8
H6	15	THR	ALA	conflict	UNP Q76PP8
H6	49	ARG	GLN	conflict	UNP Q76PP8
H6	57	ARG	GLU	conflict	UNP Q76PP8
H6	109	VAL	ILE	conflict	UNP Q76PP8
V6	15	THR	ALA	conflict	UNP Q76PP8
V6	49	ARG	GLN	conflict	UNP Q76PP8
V6	57	ARG	GLU	conflict	UNP Q76PP8
V6	109	VAL	ILE	conflict	UNP Q76PP8
W6	15	THR	ALA	conflict	UNP Q76PP8
W6	49	ARG	GLN	conflict	UNP Q76PP8
W6	57	ARG	GLU	conflict	UNP Q76PP8
W6	109	VAL	ILE	conflict	UNP Q76PP8
X6	15	THR	ALA	conflict	UNP Q76PP8
X6	49	ARG	GLN	conflict	UNP Q76PP8
X6	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
X6	109	VAL	ILE	conflict	UNP Q76PP8
Y6	15	THR	ALA	conflict	UNP Q76PP8
Y6	49	ARG	GLN	conflict	UNP Q76PP8
Y6	57	ARG	GLU	conflict	UNP Q76PP8
Y6	109	VAL	ILE	conflict	UNP Q76PP8
a7	15	THR	ALA	conflict	UNP Q76PP8
a7	49	ARG	GLN	conflict	UNP Q76PP8
a7	57	ARG	GLU	conflict	UNP Q76PP8
a7	109	VAL	ILE	conflict	UNP Q76PP8
b7	15	THR	ALA	conflict	UNP Q76PP8
b7	49	ARG	GLN	conflict	UNP Q76PP8
b7	57	ARG	GLU	conflict	UNP Q76PP8
b7	109	VAL	ILE	conflict	UNP Q76PP8
c7	15	THR	ALA	conflict	UNP Q76PP8
c7	49	ARG	GLN	conflict	UNP Q76PP8
c7	57	ARG	GLU	conflict	UNP Q76PP8
c7	109	VAL	ILE	conflict	UNP Q76PP8
d7	15	THR	ALA	conflict	UNP Q76PP8
d7	49	ARG	GLN	conflict	UNP Q76PP8
d7	57	ARG	GLU	conflict	UNP Q76PP8
d7	109	VAL	ILE	conflict	UNP Q76PP8
e7	15	THR	ALA	conflict	UNP Q76PP8
e7	49	ARG	GLN	conflict	UNP Q76PP8
e7	57	ARG	GLU	conflict	UNP Q76PP8
e7	109	VAL	ILE	conflict	UNP Q76PP8
f7	15	THR	ALA	conflict	UNP Q76PP8
f7	49	ARG	GLN	conflict	UNP Q76PP8
f7	57	ARG	GLU	conflict	UNP Q76PP8
f7	109	VAL	ILE	conflict	UNP Q76PP8
g7	15	THR	ALA	conflict	UNP Q76PP8
g7	49	ARG	GLN	conflict	UNP Q76PP8
g7	57	ARG	GLU	conflict	UNP Q76PP8
g7	109	VAL	ILE	conflict	UNP Q76PP8
h7	15	THR	ALA	conflict	UNP Q76PP8
h7	49	ARG	GLN	conflict	UNP Q76PP8
h7	57	ARG	GLU	conflict	UNP Q76PP8
h7	109	VAL	ILE	conflict	UNP Q76PP8
i7	15	THR	ALA	conflict	UNP Q76PP8
i7	49	ARG	GLN	conflict	UNP Q76PP8
i7	57	ARG	GLU	conflict	UNP Q76PP8
i7	109	VAL	ILE	conflict	UNP Q76PP8
j7	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
j7	49	ARG	GLN	conflict	UNP Q76PP8
j7	57	ARG	GLU	conflict	UNP Q76PP8
j7	109	VAL	ILE	conflict	UNP Q76PP8
k7	15	THR	ALA	conflict	UNP Q76PP8
k7	49	ARG	GLN	conflict	UNP Q76PP8
k7	57	ARG	GLU	conflict	UNP Q76PP8
k7	109	VAL	ILE	conflict	UNP Q76PP8
l7	15	THR	ALA	conflict	UNP Q76PP8
l7	49	ARG	GLN	conflict	UNP Q76PP8
l7	57	ARG	GLU	conflict	UNP Q76PP8
l7	109	VAL	ILE	conflict	UNP Q76PP8
m7	15	THR	ALA	conflict	UNP Q76PP8
m7	49	ARG	GLN	conflict	UNP Q76PP8
m7	57	ARG	GLU	conflict	UNP Q76PP8
m7	109	VAL	ILE	conflict	UNP Q76PP8
n7	15	THR	ALA	conflict	UNP Q76PP8
n7	49	ARG	GLN	conflict	UNP Q76PP8
n7	57	ARG	GLU	conflict	UNP Q76PP8
n7	109	VAL	ILE	conflict	UNP Q76PP8
o7	15	THR	ALA	conflict	UNP Q76PP8
o7	49	ARG	GLN	conflict	UNP Q76PP8
o7	57	ARG	GLU	conflict	UNP Q76PP8
o7	109	VAL	ILE	conflict	UNP Q76PP8
p7	15	THR	ALA	conflict	UNP Q76PP8
p7	49	ARG	GLN	conflict	UNP Q76PP8
p7	57	ARG	GLU	conflict	UNP Q76PP8
p7	109	VAL	ILE	conflict	UNP Q76PP8
r7	15	THR	ALA	conflict	UNP Q76PP8
r7	49	ARG	GLN	conflict	UNP Q76PP8
r7	57	ARG	GLU	conflict	UNP Q76PP8
r7	109	VAL	ILE	conflict	UNP Q76PP8
s7	15	THR	ALA	conflict	UNP Q76PP8
s7	49	ARG	GLN	conflict	UNP Q76PP8
s7	57	ARG	GLU	conflict	UNP Q76PP8
s7	109	VAL	ILE	conflict	UNP Q76PP8
t7	15	THR	ALA	conflict	UNP Q76PP8
t7	49	ARG	GLN	conflict	UNP Q76PP8
t7	57	ARG	GLU	conflict	UNP Q76PP8
t7	109	VAL	ILE	conflict	UNP Q76PP8
u7	15	THR	ALA	conflict	UNP Q76PP8
u7	49	ARG	GLN	conflict	UNP Q76PP8
u7	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
u7	109	VAL	ILE	conflict	UNP Q76PP8
v7	15	THR	ALA	conflict	UNP Q76PP8
v7	49	ARG	GLN	conflict	UNP Q76PP8
v7	57	ARG	GLU	conflict	UNP Q76PP8
v7	109	VAL	ILE	conflict	UNP Q76PP8
w7	15	THR	ALA	conflict	UNP Q76PP8
w7	49	ARG	GLN	conflict	UNP Q76PP8
w7	57	ARG	GLU	conflict	UNP Q76PP8
w7	109	VAL	ILE	conflict	UNP Q76PP8
x7	15	THR	ALA	conflict	UNP Q76PP8
x7	49	ARG	GLN	conflict	UNP Q76PP8
x7	57	ARG	GLU	conflict	UNP Q76PP8
x7	109	VAL	ILE	conflict	UNP Q76PP8
y7	15	THR	ALA	conflict	UNP Q76PP8
y7	49	ARG	GLN	conflict	UNP Q76PP8
y7	57	ARG	GLU	conflict	UNP Q76PP8
y7	109	VAL	ILE	conflict	UNP Q76PP8
a8	15	THR	ALA	conflict	UNP Q76PP8
a8	49	ARG	GLN	conflict	UNP Q76PP8
a8	57	ARG	GLU	conflict	UNP Q76PP8
a8	109	VAL	ILE	conflict	UNP Q76PP8
b8	15	THR	ALA	conflict	UNP Q76PP8
b8	49	ARG	GLN	conflict	UNP Q76PP8
b8	57	ARG	GLU	conflict	UNP Q76PP8
b8	109	VAL	ILE	conflict	UNP Q76PP8
c8	15	THR	ALA	conflict	UNP Q76PP8
c8	49	ARG	GLN	conflict	UNP Q76PP8
c8	57	ARG	GLU	conflict	UNP Q76PP8
c8	109	VAL	ILE	conflict	UNP Q76PP8
d8	15	THR	ALA	conflict	UNP Q76PP8
d8	49	ARG	GLN	conflict	UNP Q76PP8
d8	57	ARG	GLU	conflict	UNP Q76PP8
d8	109	VAL	ILE	conflict	UNP Q76PP8
e8	15	THR	ALA	conflict	UNP Q76PP8
e8	49	ARG	GLN	conflict	UNP Q76PP8
e8	57	ARG	GLU	conflict	UNP Q76PP8
e8	109	VAL	ILE	conflict	UNP Q76PP8
f8	15	THR	ALA	conflict	UNP Q76PP8
f8	49	ARG	GLN	conflict	UNP Q76PP8
f8	57	ARG	GLU	conflict	UNP Q76PP8
f8	109	VAL	ILE	conflict	UNP Q76PP8
g8	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
g8	49	ARG	GLN	conflict	UNP Q76PP8
g8	57	ARG	GLU	conflict	UNP Q76PP8
g8	109	VAL	ILE	conflict	UNP Q76PP8
h8	15	THR	ALA	conflict	UNP Q76PP8
h8	49	ARG	GLN	conflict	UNP Q76PP8
h8	57	ARG	GLU	conflict	UNP Q76PP8
h8	109	VAL	ILE	conflict	UNP Q76PP8
m8	15	THR	ALA	conflict	UNP Q76PP8
m8	49	ARG	GLN	conflict	UNP Q76PP8
m8	57	ARG	GLU	conflict	UNP Q76PP8
m8	109	VAL	ILE	conflict	UNP Q76PP8
n8	15	THR	ALA	conflict	UNP Q76PP8
n8	49	ARG	GLN	conflict	UNP Q76PP8
n8	57	ARG	GLU	conflict	UNP Q76PP8
n8	109	VAL	ILE	conflict	UNP Q76PP8
o8	15	THR	ALA	conflict	UNP Q76PP8
o8	49	ARG	GLN	conflict	UNP Q76PP8
o8	57	ARG	GLU	conflict	UNP Q76PP8
o8	109	VAL	ILE	conflict	UNP Q76PP8
p8	15	THR	ALA	conflict	UNP Q76PP8
p8	49	ARG	GLN	conflict	UNP Q76PP8
p8	57	ARG	GLU	conflict	UNP Q76PP8
p8	109	VAL	ILE	conflict	UNP Q76PP8
t8	15	THR	ALA	conflict	UNP Q76PP8
t8	49	ARG	GLN	conflict	UNP Q76PP8
t8	57	ARG	GLU	conflict	UNP Q76PP8
t8	109	VAL	ILE	conflict	UNP Q76PP8
u8	15	THR	ALA	conflict	UNP Q76PP8
u8	49	ARG	GLN	conflict	UNP Q76PP8
u8	57	ARG	GLU	conflict	UNP Q76PP8
u8	109	VAL	ILE	conflict	UNP Q76PP8
v8	15	THR	ALA	conflict	UNP Q76PP8
v8	49	ARG	GLN	conflict	UNP Q76PP8
v8	57	ARG	GLU	conflict	UNP Q76PP8
v8	109	VAL	ILE	conflict	UNP Q76PP8
w8	15	THR	ALA	conflict	UNP Q76PP8
w8	49	ARG	GLN	conflict	UNP Q76PP8
w8	57	ARG	GLU	conflict	UNP Q76PP8
w8	109	VAL	ILE	conflict	UNP Q76PP8
x8	15	THR	ALA	conflict	UNP Q76PP8
x8	49	ARG	GLN	conflict	UNP Q76PP8
x8	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
x8	109	VAL	ILE	conflict	UNP Q76PP8
y8	15	THR	ALA	conflict	UNP Q76PP8
y8	49	ARG	GLN	conflict	UNP Q76PP8
y8	57	ARG	GLU	conflict	UNP Q76PP8
y8	109	VAL	ILE	conflict	UNP Q76PP8
A9	15	THR	ALA	conflict	UNP Q76PP8
A9	49	ARG	GLN	conflict	UNP Q76PP8
A9	57	ARG	GLU	conflict	UNP Q76PP8
A9	109	VAL	ILE	conflict	UNP Q76PP8
B9	15	THR	ALA	conflict	UNP Q76PP8
B9	49	ARG	GLN	conflict	UNP Q76PP8
B9	57	ARG	GLU	conflict	UNP Q76PP8
B9	109	VAL	ILE	conflict	UNP Q76PP8
C9	15	THR	ALA	conflict	UNP Q76PP8
C9	49	ARG	GLN	conflict	UNP Q76PP8
C9	57	ARG	GLU	conflict	UNP Q76PP8
C9	109	VAL	ILE	conflict	UNP Q76PP8
D9	15	THR	ALA	conflict	UNP Q76PP8
D9	49	ARG	GLN	conflict	UNP Q76PP8
D9	57	ARG	GLU	conflict	UNP Q76PP8
D9	109	VAL	ILE	conflict	UNP Q76PP8
E9	15	THR	ALA	conflict	UNP Q76PP8
E9	49	ARG	GLN	conflict	UNP Q76PP8
E9	57	ARG	GLU	conflict	UNP Q76PP8
E9	109	VAL	ILE	conflict	UNP Q76PP8
F9	15	THR	ALA	conflict	UNP Q76PP8
F9	49	ARG	GLN	conflict	UNP Q76PP8
F9	57	ARG	GLU	conflict	UNP Q76PP8
F9	109	VAL	ILE	conflict	UNP Q76PP8
G9	15	THR	ALA	conflict	UNP Q76PP8
G9	49	ARG	GLN	conflict	UNP Q76PP8
G9	57	ARG	GLU	conflict	UNP Q76PP8
G9	109	VAL	ILE	conflict	UNP Q76PP8
H9	15	THR	ALA	conflict	UNP Q76PP8
H9	49	ARG	GLN	conflict	UNP Q76PP8
H9	57	ARG	GLU	conflict	UNP Q76PP8
H9	109	VAL	ILE	conflict	UNP Q76PP8
I9	15	THR	ALA	conflict	UNP Q76PP8
I9	49	ARG	GLN	conflict	UNP Q76PP8
I9	57	ARG	GLU	conflict	UNP Q76PP8
I9	109	VAL	ILE	conflict	UNP Q76PP8
J9	15	THR	ALA	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
J9	49	ARG	GLN	conflict	UNP Q76PP8
J9	57	ARG	GLU	conflict	UNP Q76PP8
J9	109	VAL	ILE	conflict	UNP Q76PP8
K9	15	THR	ALA	conflict	UNP Q76PP8
K9	49	ARG	GLN	conflict	UNP Q76PP8
K9	57	ARG	GLU	conflict	UNP Q76PP8
K9	109	VAL	ILE	conflict	UNP Q76PP8
L9	15	THR	ALA	conflict	UNP Q76PP8
L9	49	ARG	GLN	conflict	UNP Q76PP8
L9	57	ARG	GLU	conflict	UNP Q76PP8
L9	109	VAL	ILE	conflict	UNP Q76PP8
M9	15	THR	ALA	conflict	UNP Q76PP8
M9	49	ARG	GLN	conflict	UNP Q76PP8
M9	57	ARG	GLU	conflict	UNP Q76PP8
M9	109	VAL	ILE	conflict	UNP Q76PP8
N9	15	THR	ALA	conflict	UNP Q76PP8
N9	49	ARG	GLN	conflict	UNP Q76PP8
N9	57	ARG	GLU	conflict	UNP Q76PP8
N9	109	VAL	ILE	conflict	UNP Q76PP8
O9	15	THR	ALA	conflict	UNP Q76PP8
O9	49	ARG	GLN	conflict	UNP Q76PP8
O9	57	ARG	GLU	conflict	UNP Q76PP8
O9	109	VAL	ILE	conflict	UNP Q76PP8
P9	15	THR	ALA	conflict	UNP Q76PP8
P9	49	ARG	GLN	conflict	UNP Q76PP8
P9	57	ARG	GLU	conflict	UNP Q76PP8
P9	109	VAL	ILE	conflict	UNP Q76PP8
R9	15	THR	ALA	conflict	UNP Q76PP8
R9	49	ARG	GLN	conflict	UNP Q76PP8
R9	57	ARG	GLU	conflict	UNP Q76PP8
R9	109	VAL	ILE	conflict	UNP Q76PP8
S9	15	THR	ALA	conflict	UNP Q76PP8
S9	49	ARG	GLN	conflict	UNP Q76PP8
S9	57	ARG	GLU	conflict	UNP Q76PP8
S9	109	VAL	ILE	conflict	UNP Q76PP8
T9	15	THR	ALA	conflict	UNP Q76PP8
T9	49	ARG	GLN	conflict	UNP Q76PP8
T9	57	ARG	GLU	conflict	UNP Q76PP8
T9	109	VAL	ILE	conflict	UNP Q76PP8
U9	15	THR	ALA	conflict	UNP Q76PP8
U9	49	ARG	GLN	conflict	UNP Q76PP8
U9	57	ARG	GLU	conflict	UNP Q76PP8

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Chain	Residue	Modelled	Actual	Comment	Reference
U9	109	VAL	ILE	conflict	UNP Q76PP8
V9	15	THR	ALA	conflict	UNP Q76PP8
V9	49	ARG	GLN	conflict	UNP Q76PP8
V9	57	ARG	GLU	conflict	UNP Q76PP8
V9	109	VAL	ILE	conflict	UNP Q76PP8
W9	15	THR	ALA	conflict	UNP Q76PP8
W9	49	ARG	GLN	conflict	UNP Q76PP8
W9	57	ARG	GLU	conflict	UNP Q76PP8
W9	109	VAL	ILE	conflict	UNP Q76PP8
X9	15	THR	ALA	conflict	UNP Q76PP8
X9	49	ARG	GLN	conflict	UNP Q76PP8
X9	57	ARG	GLU	conflict	UNP Q76PP8
X9	109	VAL	ILE	conflict	UNP Q76PP8
Y9	15	THR	ALA	conflict	UNP Q76PP8
Y9	49	ARG	GLN	conflict	UNP Q76PP8
Y9	57	ARG	GLU	conflict	UNP Q76PP8
Y9	109	VAL	ILE	conflict	UNP Q76PP8

MET
 ALA
 GLY
 ARG
 SER
 GLY
 ASP
 SER
 ASP
 ASP
 GLU
 D11
 L18
 Y23
 Q24
 P28
 G33
 T34
 R58
 T62
 Y63
 L64
 G65
 R66
 ALA
 ALA
 GLU
 GLU
 PRO
 VAL
 PRO
 PRO
 LEU
 LEU
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 THR
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 ASP
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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L18 N30 P31 E32 G33 R58 I59 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY VAL GLY SER

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L18 I19 K20 Y23 Q24 P28 E32 G33 T34 R41 R59 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 V16 R17 L18 Q24 N30 P31 E32 G33 I59 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY GLN THR GLY

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L12 V16 R17 L18 I19 K20 Y23 Q24 P28 E32 G33 T34 R59 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY GLN THR GLY

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L18 P28 P29 N30 G33 T34 R58 I59 L60 S61 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY THR GLN GLY VAL

Residue	Position	Sequence	Conservation	Charge	Hydrophobicity	Volume	Weight	Mass	Order
MET	1	Met	0.00	0.00	0.00	0.00	0.00	0.00	1
ALA	2	Ala	0.00	0.00	0.00	0.00	0.00	0.00	2
GLY	3	Gly	0.00	0.00	0.00	0.00	0.00	0.00	3
ARG	4	Arg	0.00	0.00	0.00	0.00	0.00	0.00	4
SER	5	Ser	0.00	0.00	0.00	0.00	0.00	0.00	5
GLY	6	Gly	0.00	0.00	0.00	0.00	0.00	0.00	6
ASP	7	Asp	0.00	0.00	0.00	0.00	0.00	0.00	7
SER	8	Ser	0.00	0.00	0.00	0.00	0.00	0.00	8
ASP	9	Asp	0.00	0.00	0.00	0.00	0.00	0.00	9
GLU	10	Glu	0.00	0.00	0.00	0.00	0.00	0.00	10
GLU	11	Glu	0.00	0.00	0.00	0.00	0.00	0.00	11
D11	12	D11	0.00	0.00	0.00	0.00	0.00	0.00	12
T15	13	T15	0.00	0.00	0.00	0.00	0.00	0.00	13
V16	14	V16	0.00	0.00	0.00	0.00	0.00	0.00	14
E17	15	E17	0.00	0.00	0.00	0.00	0.00	0.00	15
L18	16	L18	0.00	0.00	0.00	0.00	0.00	0.00	16
Y23	17	Y23	0.00	0.00	0.00	0.00	0.00	0.00	17
P28	18	P28	0.00	0.00	0.00	0.00	0.00	0.00	18
F31	19	F31	0.00	0.00	0.00	0.00	0.00	0.00	19
E32	20	E32	0.00	0.00	0.00	0.00	0.00	0.00	20
I55	21	I55	0.00	0.00	0.00	0.00	0.00	0.00	21
S61	22	S61	0.00	0.00	0.00	0.00	0.00	0.00	22
T62	23	T62	0.00	0.00	0.00	0.00	0.00	0.00	23
Y63	24	Y63	0.00	0.00	0.00	0.00	0.00	0.00	24
L64	25	L64	0.00	0.00	0.00	0.00	0.00	0.00	25
G65	26	G65	0.00	0.00	0.00	0.00	0.00	0.00	26
R66	27	R66	0.00	0.00	0.00	0.00	0.00	0.00	27
SER	28	Ser	0.00	0.00	0.00	0.00	0.00	0.00	28
ALA	29	Ala	0.00	0.00	0.00	0.00	0.00	0.00	29
GLU	30	Glu	0.00	0.00	0.00	0.00	0.00	0.00	30
PRO	31	Pro	0.00	0.00	0.00	0.00	0.00	0.00	31
VAL	32	Val	0.00	0.00	0.00	0.00	0.00	0.00	32
PRO	33	Pro	0.00	0.00	0.00	0.00	0.00	0.00	33
PRO	34	Pro	0.00	0.00	0.00	0.00	0.00	0.00	34
LEU	35	Leu	0.00	0.00	0.00	0.00	0.00	0.00	35
LEU	36	Leu	0.00	0.00	0.00	0.00	0.00	0.00	36
PRO	37	Pro	0.00	0.00	0.00	0.00	0.00	0.00	37
LEU	38	Leu	0.00	0.00	0.00	0.00	0.00	0.00	38
ARG	39	Arg	0.00	0.00	0.00	0.00	0.00	0.00	39
GLU	40	Glu	0.00	0.00	0.00	0.00	0.00	0.00	40
LEU	41	Leu	0.00	0.00	0.00	0.00	0.00	0.00	41
THR	42	Thr	0.00	0.00	0.00	0.00	0.00	0.00	42
LEU	43	Leu	0.00	0.00	0.00	0.00	0.00	0.00	43
ASP	44	Asp	0.00	0.00	0.00	0.00	0.00	0.00	44
CYS	45	Cys	0.00	0.00	0.00	0.00	0.00	0.00	45
ASN	46	Asn	0.00	0.00	0.00	0.00	0.00	0.00	46
GLU	47	Glu	0.00	0.00	0.00</				

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 P28 E32 R35 R57 R58 I59 L60 T62 Y63 L64 G65 R66 SER ALA GLU PRO PRO VAL LEU LEU GLN PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY THR

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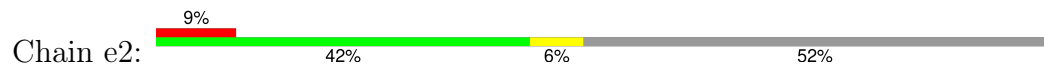
• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 R49 R53 I59 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU LEU PRO PRO LEU ARG LEU THR LEU LEU ASP CYS ASN GLU ASP CYS THR GLY THR GLN GLY VAL GLY SER PRO GLN

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 Q24 P28 P29 R30 R31 E32 G33 T34 R35 R41 R49 S61 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU GLN PRO PRO LEU ARG LEU THR LEU LEU ASP CYS ASN GLU ASP CYS THR GLY THR CYS ASN GLY VAL GLY ASP CYS GLY THR

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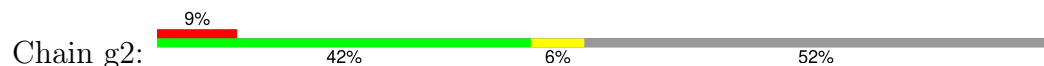
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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 R49 R53 I59 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU GLN PRO PRO LEU ARG LEU THR LEU LEU ASP CYS ASN GLU ASP CYS THR GLY THR CYS ASN GLY VAL GLY SER PRO

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 Q24 P28 P29 R30 R31 E32 G33 T34 R41 R49 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU GLN PRO PRO LEU ARG LEU THR LEU LEU ASP CYS ASN GLU ASP CYS THR GLY THR CYS ASN GLY VAL GLY SER PRO

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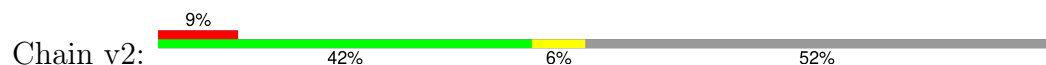
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MET ALA GLY THR ARG SER GLY ASP ASP ASP GLU D11 L18 L19 K20 Y23 Q24 P28 E32 G33 T34 R49 R58 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO PRO GLN LEU PRO PRO PRO ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP GLU D11 Y16 R17 L18 Y23 Q24 S25 P28 P29 N30 P31 E32 G33 T34 R49 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO PRO GLY THR ARG LEU THR ASP CYS ASN GLU ASP CYS GLY THR

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP GLU D11 L18 Y23 E32 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO PRO GLY THR ARG LEU THR ASP CYS ASN GLU ASP CYS GLY THR

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• Molecule 1: Protein Rev



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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP GLU D11 R17 L18 Y23 Q24 E32 G33 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO PRO GLU ARG THR LEU ASP CYS ASN GLU ASP CYS GLY THR ARG LEU THR ASP CYS GLN GLY VAL GLY SER PRO PRO GLN

Amino Acid	Number of Mutations
MET	0
ALA	10
GLY	10
ARG	10
SER	10
GLY	10
ASP	10
SER	10
ASP	10
GLU	10

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• Molecule 1: Protein Rev



MET ALA ALA GLY ARG SER GLY ASP ASP ASP D11 L12 V16 R17 L18 Y23 R49 R58 I59 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY THR GLN GLY VAL GLY
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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L12 L18 I19 K20 Y23 Q24 P28 N30 F31 E32 G33 T34 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR LEU ASP CYS ASN GLU ASP CYS THR SER
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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 L18 Q24 P28 N30 R57 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO LEU LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR LEU ASP CYS ASN GLU ASP CYS THR SER
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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP D11 Y23 Q24 N30 P31 E32 G33 T34 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR LEU ASP CYS ASN GLU ASP CYS THR SER
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MET ALA GLY ARG SER GLY ASP ASP ASP D11 Y23 Q24 P28 N30 G33 R49 R57 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR LEU ASP CYS ASN GLU ASP CYS THR SER
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• Molecule 1: Protein Rev



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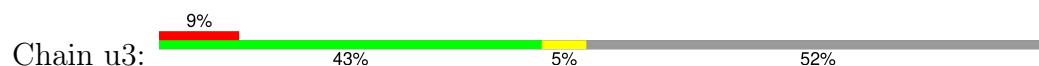
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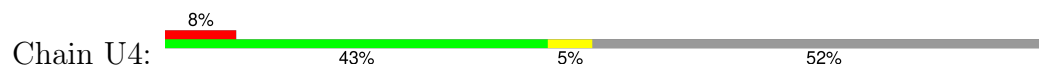
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MET ALA GLY GLN ARG SER GLY ASP ASP ASP D11 T15 V16 R17 L18 Y23 N30 P31 E32 G33 I55 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO PRO LEU LEU LEU PRO PRO LEU LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER

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MET ALA GLY GLN ARG SER GLY ASP ASP ASP D11 L12 V16 R17 L18 Y23 Q24 P28 E32 G33 T34 R46 R49 R57 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU LEU PRO PRO LEU LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER

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MET ALA GLY GLN ARG SER GLY ASP ASP ASP D11 L18 P28 G33 R49 I59 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU LEU LEU PRO PRO LEU LEU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS GLY THR SER

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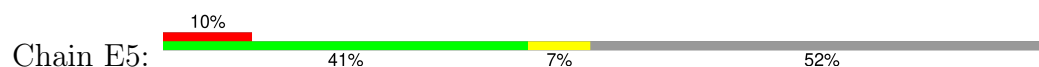
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• Molecule 1: Protein Rev



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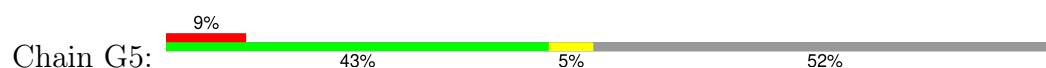
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MET ALA GLY PRO ARG SER GLN ILE LEU VAL ASP SER ASP GLU D11 V16 R17 L18 Q24 S25 P28 E32 G33 T34 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU LEU PRO CYS ASN GLU ASP CYS THR GLY THR GLN GLY

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• Molecule 1: Protein Rev



MET ALA GLY PRO ARG SER GLN ILE LEU VAL ASP SER ASP GLU D11 L12 T15 V16 R17 L18 Y23 P28 P31 E32 R49 I55 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU ASP CYS ASN GLU ASP CYS

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• Molecule 1: Protein Rev



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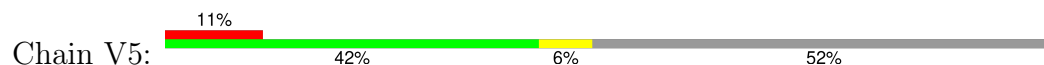
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MET ALA GLY ARG SER GLY ASP ASP ASP THR VAL L12 L18 V16 R17 Y23 Q24 E32 G33 T34 R57 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN PRO LEU LEU GLU ARG LEU THR ASP CYS ASN GLU ASP CYS GLY THR SER GLY THR GLN GLY VAL GLY

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• Molecule 1: Protein Rev



MET ALA GLY ARG SER GLY ASP ASP ASP THR VAL L12 L18 Y23 Q24 S25 P28 P29 N30 P31 E32 G33 T34 R35 R49 R58 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO GLY THR ARG LEU LEU ASP CYS ASN GLU ASP CYS GLY THR SER GLY THR GLN GLY VAL GLY THR LEU ASP CYS ASN GLU ASP CYS ASN GLU

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• Molecule 1: Protein Rev



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• Molecule 1: Protein Rev



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• Molecule 1: Protein Rev



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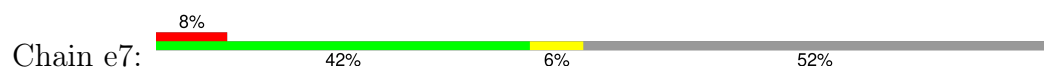
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Chain f7: 8% 47% 52%

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• Molecule 1: Protein Rev

Chain g7: 8% 44% 52%

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D11 L18 Y23 Q24 P28 E32 G33 T34 R49 S61 T62 Y63 L64 G65 R66

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• Molecule 1: Protein Rev

Chain h7: 11% 44% 52%

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• Molecule 1: Protein Rev

Chain i7: 11% 46% 52%

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• Molecule 1: Protein Rev

Chain j7: 5% 47% 52%

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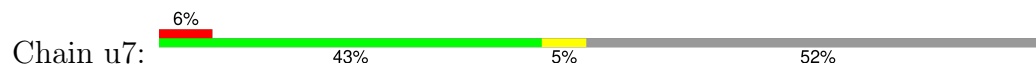
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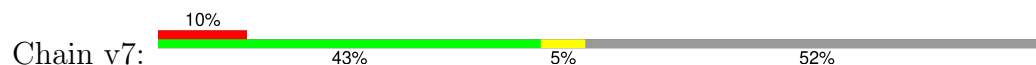
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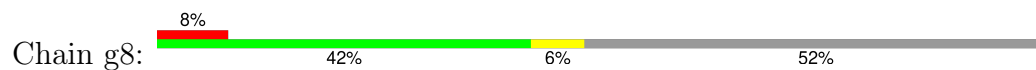


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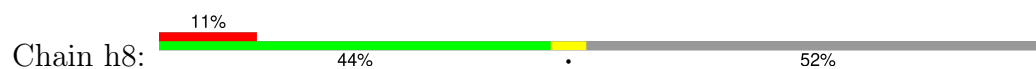
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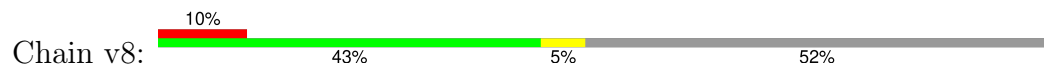
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- Molecule 1: Protein Rev



MET ALA ALA GLU D11 L18 P28 G33 R49 R58 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU LEU ASP CYS ASN ASP CYS THR SER GLY THR GLN VAL GLY

SER PRO GLN ILE VAL GLU SER PRO THR VAL LEU GLU SER GLY ALA LYS GLU

- Molecule 1: Protein Rev



MET ALA ALA GLU D11 L18 Y23 Q24 P28 E32 G33 T34 R58 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU LEU ASP CYS ASN ASP CYS THR SER GLY THR GLN VAL GLY

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MET ALA GLY ARG SER GLY ASP ASP ASP D11 V16 V17 L18 Y23 Q24 P28 P29 N30 G33 T34 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN PRO PRO PRO LEU ARG GLN THR LEU ASP CYS ASN ASP CYS THR GLY THR GLN

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MET ALA GLY ARG SER GLY ASP ASP D11 L18 Y23 G33 R49 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO GLU ARG LEU THR ASP CYS ASN ASP CYS THR GLY THR GLN VAL GLY SER PRO GLN ILE

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MET ALA GLY ARG SER GLY ASP ASP D11 L18 Y23 Q24 P28 N30 P31 E32 G33 T34 R41 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG GLU THR LEU ASP CYS ASN ASP CYS GLY THR GLN

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MET ALA GLY ARG SER GLY ASP ASP D11 L18 Y23 Q24 G33 R49 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG GLU THR LEU ASP CYS ASN ASP CYS GLY THR LEU ASP CYS VAL GLY PRO GLN

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MET ALA GLY ARG SER GLY ASP ASP D11 L12 L18 I19 K20 Y23 Q24 P28 E32 G33 T34 R35 R68 I69 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU ARG GLU THR LEU ASP CYS ASN ASP CYS GLY THR GLN

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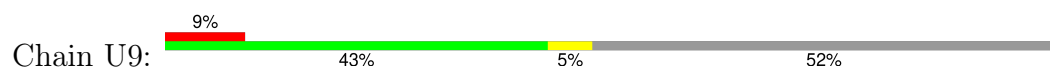
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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 I19 K20 Y23 P28 E32 G33 T34 R58 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU ASP CYS ASN ASP CYS GLY THR SER GLY

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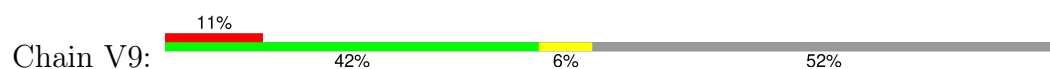
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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L12 Y16 R17 L18 Y23 Q24 P28 P29 N30 P31 E32 G33 T34 R46 R49 R57 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU ASP CYS ASN ASP CYS GLU ASP

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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 Q24 S25 P28 P29 N30 P31 E32 G33 T34 R35 Y42 R49 R58 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU ASP CYS ASN

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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L12 L18 Y23 E32 T62 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU CYS ASN ASP CYS GLY THR SER PRO GLN VAL GLY THR LEU

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MET ALA GLY ARG SER GLY ASP ASP GLU D11 L18 Y23 Q24 S25 P28 E32 G33 T34 R35 R49 R58 I59 L60 S61 T62 Y63 L64 G65 R66 SER ALA GLU PRO VAL PRO LEU GLN LEU PRO PRO LEU GLU ARG LEU THR LEU ASP CYS ASN ASP CYS GLY

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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=22°, rise=21 Å, axial sym=C6	Depositor
Number of segments used	300	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	990	Depositor
Maximum defocus (nm)	3090	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	7.224	Depositor
Minimum map value	-5.713	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.805	Depositor
Recommended contour level	1.6	Depositor
Map size (Å)	304.65, 304.65, 304.65	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0155, 1.0155, 1.0155	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	A1	0.10	0/501	0.30	0/670
1	A4	0.09	0/501	0.30	0/670
1	A5	0.10	0/501	0.31	0/670
1	A9	0.10	0/501	0.31	0/670
1	B1	0.10	0/501	0.30	0/670
1	B4	0.10	0/501	0.32	0/670
1	B5	0.10	0/501	0.31	0/670
1	B9	0.10	0/501	0.30	0/670
1	C1	0.09	0/501	0.29	0/670
1	C5	0.09	0/501	0.29	0/670
1	C6	0.10	0/501	0.30	0/670
1	C9	0.09	0/501	0.29	0/670
1	D1	0.10	0/501	0.29	0/670
1	D5	0.10	0/501	0.30	0/670
1	D6	0.09	0/501	0.29	0/670
1	D9	0.09	0/501	0.30	0/670
1	E1	0.11	0/501	0.33	0/670
1	E5	0.11	0/501	0.32	0/670
1	E6	0.11	0/501	0.32	0/670
1	E9	0.11	0/501	0.31	0/670
1	F1	0.09	0/501	0.29	0/670
1	F5	0.10	0/501	0.30	0/670
1	F6	0.09	0/501	0.30	0/670
1	F9	0.09	0/501	0.30	0/670
1	G1	0.09	0/501	0.29	0/670
1	G5	0.10	0/501	0.30	0/670
1	G6	0.10	0/501	0.30	0/670
1	G9	0.09	0/501	0.29	0/670
1	H1	0.10	0/501	0.29	0/670
1	H5	0.10	0/501	0.31	0/670
1	H6	0.10	0/501	0.30	0/670
1	H9	0.09	0/501	0.30	0/670
1	I1	0.09	0/501	0.30	0/670
1	I4	0.09	0/501	0.30	0/670

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I9	0.10	0/501	0.31	0/670
1	J1	0.09	0/501	0.30	0/670
1	J4	0.09	0/501	0.30	0/670
1	J9	0.09	0/501	0.30	0/670
1	K1	0.09	0/501	0.29	0/670
1	K4	0.09	0/501	0.29	0/670
1	K9	0.09	0/501	0.29	0/670
1	L1	0.09	0/501	0.29	0/670
1	L4	0.09	0/501	0.30	0/670
1	L9	0.09	0/501	0.30	0/670
1	M1	0.11	0/501	0.31	0/670
1	M4	0.10	0/501	0.30	0/670
1	M5	0.10	0/501	0.31	0/670
1	M9	0.11	0/501	0.31	0/670
1	N1	0.10	0/501	0.31	0/670
1	N4	0.10	0/501	0.31	0/670
1	N5	0.09	0/501	0.30	0/670
1	N9	0.10	0/501	0.32	0/670
1	O1	0.10	0/501	0.30	0/670
1	O4	0.09	0/501	0.31	0/670
1	O5	0.10	0/501	0.30	0/670
1	O9	0.10	0/501	0.30	0/670
1	P1	0.10	0/501	0.32	0/670
1	P5	0.10	0/501	0.31	0/670
1	P9	0.10	0/501	0.31	0/670
1	R1	0.09	0/501	0.29	0/670
1	R4	0.09	0/501	0.30	0/670
1	R9	0.09	0/501	0.30	0/670
1	S1	0.09	0/501	0.30	0/670
1	S4	0.09	0/501	0.30	0/670
1	S9	0.09	0/501	0.30	0/670
1	T1	0.10	0/501	0.30	0/670
1	T4	0.09	0/501	0.30	0/670
1	T5	0.10	0/501	0.31	0/670
1	T9	0.10	0/501	0.30	0/670
1	U1	0.09	0/501	0.31	0/670
1	U4	0.10	0/501	0.30	0/670
1	U5	0.10	0/501	0.30	0/670
1	U9	0.10	0/501	0.30	0/670
1	V1	0.10	0/501	0.32	0/670
1	V5	0.10	0/501	0.32	0/670
1	V6	0.10	0/501	0.32	0/670
1	V9	0.10	0/501	0.31	0/670

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	W1	0.09	0/501	0.30	0/670
1	W5	0.09	0/501	0.30	0/670
1	W6	0.09	0/501	0.30	0/670
1	W9	0.09	0/501	0.30	0/670
1	X1	0.11	0/501	0.33	0/670
1	X5	0.10	0/501	0.31	0/670
1	X6	0.11	0/501	0.33	0/670
1	X9	0.11	0/501	0.32	0/670
1	Y1	0.09	0/501	0.30	0/670
1	Y5	0.09	0/501	0.30	0/670
1	Y6	0.09	0/501	0.29	0/670
1	Y9	0.09	0/501	0.30	0/670
1	a3	0.09	0/501	0.30	0/670
1	a7	0.10	0/501	0.30	0/670
1	a8	0.10	0/501	0.31	0/670
1	b3	0.11	0/501	0.32	0/670
1	b7	0.10	0/501	0.31	0/670
1	b8	0.10	0/501	0.30	0/670
1	c2	0.09	0/501	0.30	0/670
1	c7	0.09	0/501	0.29	0/670
1	c8	0.09	0/501	0.29	0/670
1	d2	0.09	0/501	0.30	0/670
1	d7	0.09	0/501	0.30	0/670
1	d8	0.09	0/501	0.29	0/670
1	e2	0.11	0/501	0.32	0/670
1	e7	0.11	0/501	0.32	0/670
1	e8	0.11	0/501	0.32	0/670
1	f2	0.09	0/501	0.30	0/670
1	f7	0.09	0/501	0.29	0/670
1	f8	0.09	0/501	0.30	0/670
1	g2	0.10	0/501	0.29	0/670
1	g7	0.09	0/501	0.29	0/670
1	g8	0.09	0/501	0.30	0/670
1	h2	0.10	0/501	0.30	0/670
1	h7	0.09	0/501	0.30	0/670
1	h8	0.09	0/501	0.30	0/670
1	i3	0.10	0/501	0.31	0/670
1	i7	0.09	0/501	0.31	0/670
1	j3	0.10	0/501	0.30	0/670
1	j7	0.09	0/501	0.30	0/670
1	k3	0.09	0/501	0.29	0/670
1	k7	0.09	0/501	0.29	0/670
1	l3	0.09	0/501	0.29	0/670

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	l7	0.09	0/501	0.29	0/670
1	m3	0.11	0/501	0.31	0/670
1	m7	0.10	0/501	0.30	0/670
1	m8	0.11	0/501	0.31	0/670
1	n3	0.10	0/501	0.32	0/670
1	n7	0.10	0/501	0.32	0/670
1	n8	0.09	0/501	0.29	0/670
1	o3	0.09	0/501	0.29	0/670
1	o7	0.09	0/501	0.30	0/670
1	o8	0.10	0/501	0.30	0/670
1	p3	0.10	0/501	0.32	0/670
1	p7	0.10	0/501	0.31	0/670
1	p8	0.10	0/501	0.31	0/670
1	r3	0.10	0/501	0.30	0/670
1	r7	0.10	0/501	0.30	0/670
1	s3	0.09	0/501	0.30	0/670
1	s7	0.09	0/501	0.30	0/670
1	t3	0.10	0/501	0.30	0/670
1	t7	0.10	0/501	0.30	0/670
1	t8	0.10	0/501	0.31	0/670
1	u3	0.10	0/501	0.30	0/670
1	u7	0.10	0/501	0.30	0/670
1	u8	0.09	0/501	0.29	0/670
1	v2	0.10	0/501	0.32	0/670
1	v7	0.10	0/501	0.32	0/670
1	v8	0.10	0/501	0.32	0/670
1	w2	0.09	0/501	0.30	0/670
1	w7	0.09	0/501	0.30	0/670
1	w8	0.09	0/501	0.30	0/670
1	x2	0.11	0/501	0.33	0/670
1	x7	0.11	0/501	0.32	0/670
1	x8	0.09	0/501	0.31	0/670
1	y2	0.09	0/501	0.30	0/670
1	y7	0.09	0/501	0.29	0/670
1	y8	0.09	0/501	0.30	0/670
All	All	0.10	0/77655	0.30	0/103850

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	A1	492	0	521	2	0
1	A4	492	0	521	1	0
1	A5	492	0	521	2	0
1	A9	492	0	521	3	0
1	B1	492	0	521	3	0
1	B4	492	0	521	3	0
1	B5	492	0	521	3	0
1	B9	492	0	521	3	0
1	C1	492	0	521	3	0
1	C5	492	0	521	3	0
1	C6	492	0	521	3	0
1	C9	492	0	521	3	0
1	D1	492	0	521	2	0
1	D5	492	0	521	2	0
1	D6	492	0	521	1	0
1	D9	492	0	521	4	0
1	E1	492	0	521	7	0
1	E5	492	0	521	8	0
1	E6	492	0	521	7	0
1	E9	492	0	521	7	0
1	F1	492	0	521	2	0
1	F5	492	0	521	3	0
1	F6	492	0	521	1	0
1	F9	492	0	521	2	0
1	G1	492	0	521	6	0
1	G5	492	0	521	7	0
1	G6	492	0	521	7	0
1	G9	492	0	521	8	0
1	H1	492	0	521	5	0
1	H5	492	0	521	3	0
1	H6	492	0	521	4	0
1	H9	492	0	521	5	0
1	I1	492	0	521	2	0
1	I4	492	0	521	3	0
1	I9	492	0	521	3	0
1	J1	492	0	521	2	0
1	J4	492	0	521	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J9	492	0	521	2	0
1	K1	492	0	521	5	0
1	K4	492	0	521	6	0
1	K9	492	0	521	5	0
1	L1	492	0	521	3	0
1	L4	492	0	521	2	0
1	L9	492	0	521	2	0
1	M1	492	0	521	4	0
1	M4	492	0	521	4	0
1	M5	492	0	521	3	0
1	M9	492	0	521	4	0
1	N1	492	0	521	2	0
1	N4	492	0	521	2	0
1	N5	492	0	521	1	0
1	N9	492	0	521	2	0
1	O1	492	0	521	2	0
1	O4	492	0	521	0	0
1	O5	492	0	521	2	0
1	O9	492	0	521	2	0
1	P1	492	0	521	2	0
1	P5	492	0	521	4	0
1	P9	492	0	521	4	0
1	R1	492	0	521	2	0
1	R4	492	0	521	2	0
1	R9	492	0	521	2	0
1	S1	492	0	521	2	0
1	S4	492	0	521	2	0
1	S9	492	0	521	2	0
1	T1	492	0	521	2	0
1	T4	492	0	521	1	0
1	T5	492	0	521	2	0
1	T9	492	0	521	2	0
1	U1	492	0	521	4	0
1	U4	492	0	521	6	0
1	U5	492	0	521	3	0
1	U9	492	0	521	6	0
1	V1	492	0	521	6	0
1	V5	492	0	521	7	0
1	V6	492	0	521	6	0
1	V9	492	0	521	7	0
1	W1	492	0	521	1	0
1	W5	492	0	521	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W6	492	0	521	2	0
1	W9	492	0	521	2	0
1	X1	492	0	521	4	0
1	X5	492	0	521	4	0
1	X6	492	0	521	4	0
1	X9	492	0	521	4	0
1	Y1	492	0	521	3	0
1	Y5	492	0	521	2	0
1	Y6	492	0	521	2	0
1	Y9	492	0	521	2	0
1	a3	492	0	521	1	0
1	a7	492	0	521	2	0
1	a8	492	0	521	2	0
1	b3	492	0	521	3	0
1	b7	492	0	521	3	0
1	b8	492	0	521	3	0
1	c2	492	0	521	3	0
1	c7	492	0	521	3	0
1	c8	492	0	521	3	0
1	d2	492	0	521	1	0
1	d7	492	0	521	4	0
1	d8	492	0	521	2	0
1	e2	492	0	521	7	0
1	e7	492	0	521	7	0
1	e8	492	0	521	7	0
1	f2	492	0	521	1	0
1	f7	492	0	521	2	0
1	f8	492	0	521	2	0
1	g2	492	0	521	7	0
1	g7	492	0	521	6	0
1	g8	492	0	521	7	0
1	h2	492	0	521	3	0
1	h7	492	0	521	5	0
1	h8	492	0	521	5	0
1	i3	492	0	521	3	0
1	i7	492	0	521	3	0
1	j3	492	0	521	2	0
1	j7	492	0	521	2	0
1	k3	492	0	521	5	0
1	k7	492	0	521	5	0
1	l3	492	0	521	4	0
1	l7	492	0	521	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	m3	492	0	521	4	0
1	m7	492	0	521	4	0
1	m8	492	0	521	3	0
1	n3	492	0	521	2	0
1	n7	492	0	521	2	0
1	n8	492	0	521	1	0
1	o3	492	0	521	0	0
1	o7	492	0	521	2	0
1	o8	492	0	521	2	0
1	p3	492	0	521	1	0
1	p7	492	0	521	4	0
1	p8	492	0	521	3	0
1	r3	492	0	521	2	0
1	r7	492	0	521	2	0
1	s3	492	0	521	2	0
1	s7	492	0	521	2	0
1	t3	492	0	521	2	0
1	t7	492	0	521	2	0
1	t8	492	0	521	2	0
1	u3	492	0	521	6	0
1	u7	492	0	521	6	0
1	u8	492	0	521	3	0
1	v2	492	0	521	6	0
1	v7	492	0	521	6	0
1	v8	492	0	521	6	0
1	w2	492	0	521	2	0
1	w7	492	0	521	2	0
1	w8	492	0	521	2	0
1	x2	492	0	521	4	0
1	x7	492	0	521	4	0
1	x8	492	0	521	4	0
1	y2	492	0	521	2	0
1	y7	492	0	521	3	0
1	y8	492	0	521	2	0
All	All	76260	0	80755	278	0

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

All (278) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B9:28:PRO:HB2	1:M9:28:PRO:HB2	1.78	0.65
1:B5:28:PRO:HB2	1:M5:28:PRO:HB2	1.78	0.65
1:b8:28:PRO:HB2	1:m8:28:PRO:HB2	1.78	0.65
1:C6:28:PRO:HB2	1:H6:28:PRO:HB2	1.79	0.65
1:B4:28:PRO:HB2	1:M4:28:PRO:HB2	1.79	0.64
1:c2:28:PRO:HB2	1:h2:28:PRO:HB2	1.79	0.64
1:C1:28:PRO:HB2	1:H1:28:PRO:HB2	1.79	0.64
1:b3:28:PRO:HB2	1:m3:28:PRO:HB2	1.78	0.64
1:B1:28:PRO:HB2	1:M1:28:PRO:HB2	1.78	0.64
1:c7:28:PRO:HB2	1:h7:28:PRO:HB2	1.79	0.64
1:b7:28:PRO:HB2	1:m7:28:PRO:HB2	1.79	0.63
1:D9:28:PRO:HB2	1:O9:28:PRO:HB2	1.80	0.63
1:c8:28:PRO:HB2	1:h8:28:PRO:HB2	1.79	0.63
1:C5:28:PRO:HB2	1:H5:28:PRO:HB2	1.79	0.63
1:d8:28:PRO:HB2	1:o8:28:PRO:HB2	1.80	0.63
1:D5:28:PRO:HB2	1:O5:28:PRO:HB2	1.80	0.63
1:D1:28:PRO:HB2	1:O1:28:PRO:HB2	1.80	0.62
1:C9:28:PRO:HB2	1:H9:28:PRO:HB2	1.80	0.62
1:d7:28:PRO:HB2	1:o7:28:PRO:HB2	1.80	0.62
1:e2:30:ASN:HD21	1:x2:49:ARG:HH12	1.49	0.61
1:e8:30:ASN:HD21	1:x8:49:ARG:HH12	1.48	0.61
1:E1:30:ASN:HD21	1:X1:49:ARG:HH12	1.49	0.60
1:e7:30:ASN:HD21	1:x7:49:ARG:HH12	1.49	0.60
1:E6:30:ASN:HD21	1:X6:49:ARG:HH12	1.49	0.59
1:H1:16:VAL:HG21	1:h8:12:LEU:HD11	1.85	0.59
1:H1:12:LEU:HD11	1:h8:16:VAL:HG21	1.85	0.59
1:K4:28:PRO:HB2	1:U4:28:PRO:HB2	1.85	0.59
1:E5:30:ASN:HD21	1:X5:49:ARG:HH12	1.49	0.59
1:k7:28:PRO:HB2	1:u7:28:PRO:HB2	1.85	0.59
1:E9:30:ASN:HD21	1:X9:49:ARG:HH12	1.49	0.59
1:K1:28:PRO:HB2	1:U1:28:PRO:HB2	1.84	0.58
1:k3:28:PRO:HB2	1:u3:28:PRO:HB2	1.85	0.58
1:K9:28:PRO:HB2	1:U9:28:PRO:HB2	1.84	0.58
1:G6:28:PRO:HB2	1:V6:28:PRO:HB2	1.86	0.58
1:G1:28:PRO:HB2	1:V1:28:PRO:HB2	1.86	0.57
1:k7:18:LEU:HD13	1:l7:18:LEU:HD21	1.86	0.57
1:G1:18:LEU:HD13	1:H1:18:LEU:HD21	1.86	0.57
1:g7:28:PRO:HB2	1:v7:28:PRO:HB2	1.87	0.57
1:g2:18:LEU:HD13	1:h2:18:LEU:HD21	1.86	0.57
1:o7:18:LEU:HD13	1:p7:18:LEU:HD21	1.87	0.57
1:K1:18:LEU:HD13	1:L1:18:LEU:HD21	1.87	0.57
1:g2:28:PRO:HB2	1:v2:28:PRO:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c7:18:LEU:HD13	1:d7:18:LEU:HD21	1.87	0.57
1:G6:18:LEU:HD13	1:H6:18:LEU:HD21	1.86	0.57
1:O1:18:LEU:HD13	1:P1:18:LEU:HD21	1.87	0.56
1:G5:28:PRO:HB2	1:V5:28:PRO:HB2	1.87	0.56
1:C9:18:LEU:HD13	1:D9:18:LEU:HD21	1.88	0.56
1:C1:18:LEU:HD13	1:D1:18:LEU:HD21	1.88	0.56
1:A9:28:PRO:HB2	1:F9:28:PRO:HB2	1.88	0.56
1:g8:28:PRO:HB2	1:v8:28:PRO:HB2	1.86	0.56
1:O9:18:LEU:HD13	1:P9:18:LEU:HD21	1.86	0.56
1:G5:18:LEU:HD13	1:H5:18:LEU:HD21	1.87	0.56
1:G9:28:PRO:HB2	1:V9:28:PRO:HB2	1.86	0.56
1:a8:28:PRO:HB2	1:f8:28:PRO:HB2	1.88	0.55
1:a8:18:LEU:HD13	1:b8:18:LEU:HD21	1.87	0.55
1:G9:18:LEU:HD13	1:H9:18:LEU:HD21	1.89	0.55
1:I1:18:LEU:HD13	1:J1:18:LEU:HD21	1.88	0.55
1:k3:18:LEU:HD13	1:l3:18:LEU:HD21	1.88	0.55
1:A5:28:PRO:HB2	1:F5:28:PRO:HB2	1.88	0.55
1:a7:28:PRO:HB2	1:f7:28:PRO:HB2	1.89	0.55
1:g8:18:LEU:HD13	1:h8:18:LEU:HD21	1.87	0.55
1:p7:12:LEU:HD11	1:D9:16:VAL:HG21	1.89	0.55
1:X9:18:LEU:HD13	1:Y9:18:LEU:HD21	1.88	0.55
1:T1:18:LEU:HD13	1:U1:18:LEU:HD21	1.89	0.55
1:T5:18:LEU:HD13	1:U5:18:LEU:HD21	1.89	0.55
1:A5:18:LEU:HD13	1:B5:18:LEU:HD21	1.88	0.54
1:a7:18:LEU:HD13	1:b7:18:LEU:HD21	1.88	0.54
1:K9:18:LEU:HD13	1:L9:18:LEU:HD21	1.89	0.54
1:A1:18:LEU:HD13	1:B1:18:LEU:HD21	1.88	0.54
1:l3:12:LEU:HD11	1:P5:16:VAL:HG21	1.88	0.54
1:g7:18:LEU:HD13	1:h7:18:LEU:HD21	1.88	0.54
1:c8:18:LEU:HD13	1:d8:18:LEU:HD21	1.88	0.54
1:v8:18:LEU:HD13	1:w8:18:LEU:HD21	1.90	0.54
1:t3:18:LEU:HD13	1:u3:18:LEU:HD21	1.90	0.54
1:T9:18:LEU:HD13	1:U9:18:LEU:HD21	1.90	0.54
1:A1:28:PRO:HB2	1:F1:28:PRO:HB2	1.89	0.54
1:t7:18:LEU:HD13	1:u7:18:LEU:HD21	1.90	0.54
1:V1:18:LEU:HD13	1:W1:18:LEU:HD21	1.90	0.53
1:x8:18:LEU:HD13	1:y8:18:LEU:HD21	1.90	0.53
1:E6:49:ARG:NH1	1:X6:32:GLU:OE2	2.42	0.53
1:E9:49:ARG:NH1	1:X9:32:GLU:OE2	2.41	0.53
1:e2:49:ARG:NH1	1:x2:32:GLU:OE2	2.42	0.53
1:V6:18:LEU:HD13	1:W6:18:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:t8:18:LEU:HD13	1:u8:18:LEU:HD21	1.90	0.53
1:v2:18:LEU:HD13	1:w2:18:LEU:HD21	1.91	0.53
1:C5:18:LEU:HD13	1:D5:18:LEU:HD21	1.89	0.53
1:e8:18:LEU:HD13	1:f8:18:LEU:HD21	1.91	0.53
1:e8:49:ARG:NH1	1:x8:32:GLU:OE2	2.42	0.53
1:o8:18:LEU:HD13	1:p8:18:LEU:HD21	1.91	0.53
1:C6:18:LEU:HD13	1:D6:18:LEU:HD21	1.91	0.53
1:E1:49:ARG:NH1	1:X1:32:GLU:OE2	2.42	0.52
1:l3:16:VAL:HG21	1:P5:12:LEU:HD11	1.90	0.52
1:K4:18:LEU:HD13	1:L4:18:LEU:HD21	1.92	0.52
1:e7:49:ARG:NH1	1:x7:32:GLU:OE2	2.42	0.52
1:i3:28:PRO:HB2	1:s3:28:PRO:HB2	1.91	0.52
1:I9:28:PRO:HB2	1:S9:28:PRO:HB2	1.91	0.52
1:x2:18:LEU:HD13	1:y2:18:LEU:HD21	1.91	0.52
1:u3:16:VAL:HG21	1:U5:12:LEU:HD11	1.92	0.52
1:i7:28:PRO:HB2	1:s7:28:PRO:HB2	1.91	0.52
1:I1:28:PRO:HB2	1:S1:28:PRO:HB2	1.91	0.52
1:u3:12:LEU:HD11	1:U5:16:VAL:HG21	1.90	0.52
1:O5:18:LEU:HD13	1:P5:18:LEU:HD21	1.91	0.52
1:X5:18:LEU:HD13	1:Y5:18:LEU:HD21	1.91	0.52
1:E5:49:ARG:NH1	1:X5:32:GLU:OE2	2.42	0.52
1:X6:18:LEU:HD13	1:Y6:18:LEU:HD21	1.91	0.52
1:E9:18:LEU:HD13	1:F9:18:LEU:HD21	1.92	0.52
1:h7:12:LEU:HD11	1:U9:16:VAL:HG21	1.91	0.52
1:v7:18:LEU:HD13	1:w7:18:LEU:HD21	1.91	0.52
1:X1:18:LEU:HD13	1:Y1:18:LEU:HD21	1.91	0.51
1:h7:16:VAL:HG21	1:U9:12:LEU:HD11	1.92	0.51
1:I4:28:PRO:HB2	1:S4:28:PRO:HB2	1.91	0.51
1:I4:16:VAL:HG21	1:m7:12:LEU:HD21	1.92	0.51
1:d7:16:VAL:HG21	1:P9:12:LEU:HD11	1.91	0.51
1:e2:28:PRO:HB2	1:x2:28:PRO:HB2	1.94	0.50
1:A9:18:LEU:HD13	1:B9:18:LEU:HD21	1.93	0.50
1:c2:18:LEU:HD13	1:d2:18:LEU:HD21	1.92	0.50
1:x7:18:LEU:HD13	1:y7:18:LEU:HD21	1.91	0.50
1:E9:23:TYR:HE1	1:E9:49:ARG:HE	1.59	0.50
1:P1:28:PRO:HB2	1:T1:28:PRO:HB2	1.92	0.50
1:E5:18:LEU:HD13	1:F5:18:LEU:HD21	1.93	0.50
1:V9:18:LEU:HD13	1:W9:18:LEU:HD21	1.93	0.50
1:p7:28:PRO:HB2	1:t7:28:PRO:HB2	1.93	0.50
1:g7:49:ARG:NH1	1:v7:32:GLU:OE2	2.45	0.49
1:p7:16:VAL:HG21	1:D9:12:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E1:28:PRO:HB2	1:X1:28:PRO:HB2	1.94	0.49
1:M5:18:LEU:HD13	1:N5:18:LEU:HD21	1.94	0.49
1:k3:32:GLU:OE2	1:u3:49:ARG:NH1	2.46	0.49
1:T4:18:LEU:HD13	1:U4:18:LEU:HD21	1.93	0.49
1:G5:49:ARG:NH1	1:V5:32:GLU:OE2	2.45	0.49
1:G6:49:ARG:NH1	1:V6:32:GLU:OE2	2.45	0.49
1:g8:49:ARG:NH1	1:v8:32:GLU:OE2	2.45	0.49
1:V1:23:TYR:HE1	1:V1:49:ARG:HE	1.61	0.49
1:P5:28:PRO:HB2	1:T5:28:PRO:HB2	1.94	0.49
1:p8:28:PRO:HB2	1:t8:28:PRO:HB2	1.94	0.49
1:P9:28:PRO:HB2	1:T9:28:PRO:HB2	1.93	0.49
1:E6:28:PRO:HB2	1:X6:28:PRO:HB2	1.94	0.49
1:k7:32:GLU:OE2	1:u7:49:ARG:NH1	2.46	0.49
1:m8:18:LEU:HD13	1:n8:18:LEU:HD21	1.94	0.49
1:E9:28:PRO:HB2	1:X9:28:PRO:HB2	1.94	0.49
1:G9:49:ARG:NH1	1:V9:32:GLU:OE2	2.45	0.49
1:g2:49:ARG:NH1	1:v2:32:GLU:OE2	2.45	0.49
1:i3:16:VAL:HG21	1:M9:12:LEU:HD21	1.93	0.49
1:M4:18:LEU:HD13	1:N4:18:LEU:HD21	1.95	0.49
1:K9:32:GLU:OE2	1:U9:49:ARG:NH1	2.46	0.49
1:e7:28:PRO:HB2	1:x7:28:PRO:HB2	1.94	0.48
1:G9:23:TYR:HE1	1:G9:49:ARG:HE	1.61	0.48
1:v2:23:TYR:HE1	1:v2:49:ARG:HE	1.62	0.48
1:m3:18:LEU:HD13	1:n3:18:LEU:HD21	1.96	0.48
1:G1:23:TYR:HE1	1:G1:49:ARG:HE	1.60	0.48
1:r3:18:LEU:HD13	1:s3:18:LEU:HD21	1.96	0.48
1:V6:23:TYR:HE1	1:V6:49:ARG:HE	1.61	0.48
1:e8:28:PRO:HB2	1:x8:28:PRO:HB2	1.94	0.48
1:G1:49:ARG:NH1	1:V1:32:GLU:OE2	2.46	0.48
1:m7:18:LEU:HD13	1:n7:18:LEU:HD21	1.96	0.48
1:r7:18:LEU:HD13	1:s7:18:LEU:HD21	1.96	0.48
1:g7:23:TYR:HE1	1:g7:49:ARG:HE	1.62	0.48
1:p3:28:PRO:HB2	1:t3:28:PRO:HB2	1.94	0.48
1:v8:23:TYR:HE1	1:v8:49:ARG:HE	1.61	0.48
1:M9:18:LEU:HD13	1:N9:18:LEU:HD21	1.96	0.48
1:K1:32:GLU:OE2	1:U1:49:ARG:NH1	2.47	0.48
1:Y1:28:PRO:HB2	1:J4:28:PRO:HB2	1.95	0.48
1:g8:23:TYR:HE1	1:g8:49:ARG:HE	1.61	0.48
1:E6:18:LEU:HD13	1:F6:18:LEU:HD21	1.96	0.48
1:W6:32:GLU:OE1	1:L9:49:ARG:NH1	2.47	0.48
1:R4:18:LEU:HD13	1:S4:18:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v7:23:TYR:HE1	1:v7:49:ARG:HE	1.62	0.47
1:R9:18:LEU:HD13	1:S9:18:LEU:HD21	1.96	0.47
1:M1:18:LEU:HD13	1:N1:18:LEU:HD21	1.96	0.47
1:e2:18:LEU:HD13	1:f2:18:LEU:HD21	1.96	0.47
1:A4:18:LEU:HD13	1:B4:18:LEU:HD21	1.96	0.47
1:V5:23:TYR:HE1	1:V5:49:ARG:HE	1.63	0.47
1:I4:18:LEU:HD13	1:J4:18:LEU:HD21	1.96	0.47
1:E5:28:PRO:HB2	1:X5:28:PRO:HB2	1.94	0.47
1:G5:23:TYR:HE1	1:G5:49:ARG:HE	1.63	0.47
1:V5:18:LEU:HD13	1:W5:18:LEU:HD21	1.96	0.47
1:I9:18:LEU:HD13	1:J9:18:LEU:HD21	1.96	0.47
1:V9:23:TYR:HE1	1:V9:49:ARG:HE	1.63	0.47
1:E5:23:TYR:HE1	1:E5:49:ARG:HE	1.63	0.47
1:K4:32:GLU:OE2	1:U4:49:ARG:NH1	2.47	0.47
1:d7:12:LEU:HD11	1:P9:16:VAL:HG21	1.97	0.47
1:i3:18:LEU:HD13	1:j3:18:LEU:HD21	1.96	0.47
1:m3:12:LEU:HD21	1:I9:16:VAL:HG21	1.96	0.47
1:E1:18:LEU:HD13	1:F1:18:LEU:HD21	1.97	0.47
1:L4:12:LEU:HD11	1:p8:16:VAL:HG21	1.97	0.47
1:G5:32:GLU:OE2	1:V5:49:ARG:NH1	2.48	0.47
1:c8:32:GLU:OE2	1:h8:49:ARG:NH1	2.48	0.47
1:G9:32:GLU:OE2	1:V9:49:ARG:NH1	2.48	0.47
1:e7:18:LEU:HD13	1:f7:18:LEU:HD21	1.97	0.46
1:e8:23:TYR:HE1	1:e8:49:ARG:HE	1.63	0.46
1:e8:29:PRO:HB2	1:e8:41:ARG:HD3	1.98	0.46
1:G1:32:GLU:OE2	1:V1:49:ARG:NH1	2.49	0.46
1:G6:23:TYR:HE1	1:G6:49:ARG:HE	1.64	0.46
1:C1:32:GLU:OE2	1:H1:49:ARG:NH1	2.48	0.46
1:c2:32:GLU:OE2	1:h2:49:ARG:NH1	2.48	0.46
1:g7:32:GLU:OE2	1:v7:49:ARG:NH1	2.48	0.46
1:E1:23:TYR:HE1	1:E1:49:ARG:HE	1.63	0.46
1:w2:32:GLU:OE1	1:l7:49:ARG:NH1	2.49	0.46
1:g8:32:GLU:OE2	1:v8:49:ARG:NH1	2.48	0.46
1:e2:23:TYR:HE1	1:e2:49:ARG:HE	1.63	0.46
1:g2:30:ASN:O	1:g2:41:ARG:NH1	2.47	0.46
1:i7:18:LEU:HD13	1:j7:18:LEU:HD21	1.96	0.46
1:a3:18:LEU:HD13	1:b3:18:LEU:HD21	1.97	0.46
1:R1:18:LEU:HD13	1:S1:18:LEU:HD21	1.97	0.46
1:U4:12:LEU:HD11	1:u8:16:VAL:HG21	1.98	0.46
1:G9:30:ASN:O	1:G9:41:ARG:NH1	2.47	0.45
1:g2:23:TYR:HE1	1:g2:49:ARG:HE	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:32:GLU:HG2	1:U4:46:ARG:HG2	1.99	0.45
1:E6:23:TYR:HE1	1:E6:49:ARG:HE	1.63	0.45
1:G6:32:GLU:OE2	1:V6:49:ARG:NH1	2.49	0.45
1:K1:32:GLU:HG2	1:U1:46:ARG:HG2	1.98	0.45
1:E5:29:PRO:HB2	1:E5:41:ARG:HD3	1.98	0.45
1:C9:32:GLU:OE2	1:H9:49:ARG:NH1	2.50	0.45
1:g2:32:GLU:OE2	1:v2:49:ARG:NH1	2.50	0.45
1:C6:32:GLU:OE2	1:H6:49:ARG:NH1	2.48	0.45
1:E1:29:PRO:HB2	1:E1:41:ARG:HD3	1.99	0.45
1:e2:29:PRO:HB2	1:e2:41:ARG:HD3	1.99	0.45
1:e7:23:TYR:HE1	1:e7:49:ARG:HE	1.63	0.45
1:E6:29:PRO:HB2	1:E6:41:ARG:HD3	1.99	0.45
1:c7:32:GLU:OE2	1:h7:49:ARG:NH1	2.50	0.45
1:e7:29:PRO:HB2	1:e7:41:ARG:HD3	1.99	0.45
1:E9:29:PRO:HB2	1:E9:41:ARG:HD3	1.98	0.45
1:n3:28:PRO:HB2	1:r3:28:PRO:HB2	2.00	0.44
1:e7:30:ASN:O	1:e7:41:ARG:NH1	2.48	0.44
1:n7:28:PRO:HB2	1:r7:28:PRO:HB2	1.99	0.44
1:C5:32:GLU:OE2	1:H5:49:ARG:NH1	2.50	0.44
1:N9:28:PRO:HB2	1:R9:28:PRO:HB2	1.99	0.44
1:E1:30:ASN:O	1:E1:41:ARG:NH1	2.48	0.44
1:L1:32:GLU:OE1	1:j3:49:ARG:NH1	2.51	0.44
1:u7:16:VAL:HG21	1:H9:12:LEU:HD11	1.99	0.44
1:N4:28:PRO:HB2	1:R4:28:PRO:HB2	1.99	0.44
1:E6:30:ASN:O	1:E6:41:ARG:NH1	2.48	0.44
1:E5:16:VAL:HG11	1:H6:64:LEU:HD13	2.00	0.43
1:M1:16:VAL:HG21	1:V5:12:LEU:HD21	1.99	0.43
1:E5:30:ASN:O	1:E5:41:ARG:NH1	2.50	0.43
1:g8:30:ASN:O	1:g8:41:ARG:NH1	2.47	0.43
1:K9:32:GLU:HG2	1:U9:46:ARG:HG2	2.01	0.43
1:U4:16:VAL:HG21	1:u8:12:LEU:HD11	2.00	0.43
1:k7:32:GLU:HG2	1:u7:46:ARG:HG2	2.01	0.43
1:u7:12:LEU:HD11	1:H9:16:VAL:HG21	2.00	0.43
1:k3:32:GLU:HG2	1:u3:46:ARG:HG2	2.01	0.43
1:g7:49:ARG:HH12	1:v7:30:ASN:HD21	1.67	0.43
1:Y1:32:GLU:OE1	1:J4:49:ARG:NH1	2.52	0.43
1:Y5:49:ARG:NH1	1:w7:32:GLU:OE1	2.52	0.43
1:g8:49:ARG:HH12	1:v8:30:ASN:HD21	1.67	0.43
1:K9:32:GLU:O	1:K9:41:ARG:NH1	2.52	0.43
1:y2:32:GLU:OE1	1:j7:49:ARG:NH1	2.52	0.42
1:K1:32:GLU:O	1:K1:41:ARG:NH1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E9:30:ASN:O	1:E9:41:ARG:NH1	2.49	0.42
1:G5:49:ARG:HH12	1:V5:30:ASN:HD21	1.67	0.42
1:G6:49:ARG:HH12	1:V6:30:ASN:HD21	1.68	0.42
1:B9:49:ARG:NH1	1:M9:32:GLU:OE2	2.53	0.42
1:N1:28:PRO:HB2	1:R1:28:PRO:HB2	2.02	0.42
1:G6:30:ASN:O	1:G6:41:ARG:NH1	2.47	0.42
1:e2:30:ASN:O	1:e2:41:ARG:NH1	2.48	0.42
1:w8:32:GLU:OE1	1:Y9:49:ARG:NH1	2.52	0.42
1:G1:49:ARG:HH12	1:V1:30:ASN:HD21	1.68	0.42
1:W5:49:ARG:NH1	1:y7:32:GLU:OE1	2.53	0.42
1:b8:49:ARG:NH1	1:m8:32:GLU:OE2	2.53	0.42
1:B1:49:ARG:NH1	1:M1:32:GLU:OE2	2.53	0.41
1:b7:49:ARG:NH1	1:m7:32:GLU:OE2	2.53	0.41
1:y8:49:ARG:NH1	1:W9:32:GLU:OE1	2.53	0.41
1:L1:16:VAL:HG11	1:A9:12:LEU:HD21	2.01	0.41
1:b3:49:ARG:NH1	1:m3:32:GLU:OE2	2.53	0.41
1:Y6:32:GLU:OE1	1:J9:49:ARG:NH1	2.53	0.41
1:B4:49:ARG:NH1	1:M4:32:GLU:OE2	2.54	0.41
1:k7:32:GLU:O	1:k7:41:ARG:NH1	2.52	0.41
1:J1:32:GLU:OE1	1:l3:49:ARG:NH1	2.54	0.41
1:W5:32:GLU:OE1	1:y7:49:ARG:NH1	2.54	0.41
1:e8:30:ASN:O	1:e8:41:ARG:NH1	2.50	0.41
1:B5:49:ARG:NH1	1:M5:32:GLU:OE2	2.53	0.41
1:F5:16:VAL:HG11	1:G5:12:LEU:HD21	2.03	0.41
1:G9:38:ARG:HE	1:V9:42:ARG:HH11	1.69	0.41
1:G9:49:ARG:HH12	1:V9:30:ASN:HD21	1.68	0.41
1:k3:32:GLU:O	1:k3:41:ARG:NH1	2.52	0.40
1:g2:49:ARG:HH12	1:v2:30:ASN:HD21	1.68	0.40
1:K4:32:GLU:O	1:K4:41:ARG:NH1	2.51	0.40
1:M4:12:LEU:HD21	1:i7:16:VAL:HG21	2.03	0.40
1:K4:29:PRO:HB2	1:K4:41:ARG:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	A4	54/116 (47%)	54 (100%)	0	0	100	100
1	A5	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	A9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	B1	54/116 (47%)	54 (100%)	0	0	100	100
1	B4	54/116 (47%)	54 (100%)	0	0	100	100
1	B5	54/116 (47%)	54 (100%)	0	0	100	100
1	B9	54/116 (47%)	54 (100%)	0	0	100	100
1	C1	54/116 (47%)	54 (100%)	0	0	100	100
1	C5	54/116 (47%)	54 (100%)	0	0	100	100
1	C6	54/116 (47%)	54 (100%)	0	0	100	100
1	C9	54/116 (47%)	54 (100%)	0	0	100	100
1	D1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	D5	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	D6	54/116 (47%)	54 (100%)	0	0	100	100
1	D9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	E1	54/116 (47%)	54 (100%)	0	0	100	100
1	E5	54/116 (47%)	54 (100%)	0	0	100	100
1	E6	54/116 (47%)	54 (100%)	0	0	100	100
1	E9	54/116 (47%)	54 (100%)	0	0	100	100
1	F1	54/116 (47%)	54 (100%)	0	0	100	100
1	F5	54/116 (47%)	54 (100%)	0	0	100	100
1	F6	54/116 (47%)	54 (100%)	0	0	100	100
1	F9	54/116 (47%)	54 (100%)	0	0	100	100
1	G1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	G5	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	G6	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	G9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	H1	54/116 (47%)	54 (100%)	0	0	100	100
1	H5	54/116 (47%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H6	54/116 (47%)	54 (100%)	0	0	100	100
1	H9	54/116 (47%)	54 (100%)	0	0	100	100
1	I1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	I4	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	I9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	J1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	J4	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	J9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	K1	54/116 (47%)	54 (100%)	0	0	100	100
1	K4	54/116 (47%)	54 (100%)	0	0	100	100
1	K9	54/116 (47%)	54 (100%)	0	0	100	100
1	L1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	L4	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	L9	54/116 (47%)	54 (100%)	0	0	100	100
1	M1	54/116 (47%)	54 (100%)	0	0	100	100
1	M4	54/116 (47%)	54 (100%)	0	0	100	100
1	M5	54/116 (47%)	54 (100%)	0	0	100	100
1	M9	54/116 (47%)	54 (100%)	0	0	100	100
1	N1	54/116 (47%)	54 (100%)	0	0	100	100
1	N4	54/116 (47%)	54 (100%)	0	0	100	100
1	N5	54/116 (47%)	54 (100%)	0	0	100	100
1	N9	54/116 (47%)	54 (100%)	0	0	100	100
1	O1	54/116 (47%)	54 (100%)	0	0	100	100
1	O4	54/116 (47%)	54 (100%)	0	0	100	100
1	O5	54/116 (47%)	54 (100%)	0	0	100	100
1	O9	54/116 (47%)	54 (100%)	0	0	100	100
1	P1	54/116 (47%)	54 (100%)	0	0	100	100
1	P5	54/116 (47%)	54 (100%)	0	0	100	100
1	P9	54/116 (47%)	54 (100%)	0	0	100	100
1	R1	54/116 (47%)	54 (100%)	0	0	100	100
1	R4	54/116 (47%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R9	54/116 (47%)	54 (100%)	0	0	100	100
1	S1	54/116 (47%)	54 (100%)	0	0	100	100
1	S4	54/116 (47%)	54 (100%)	0	0	100	100
1	S9	54/116 (47%)	54 (100%)	0	0	100	100
1	T1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	T4	54/116 (47%)	54 (100%)	0	0	100	100
1	T5	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	T9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	U1	54/116 (47%)	54 (100%)	0	0	100	100
1	U4	54/116 (47%)	54 (100%)	0	0	100	100
1	U5	54/116 (47%)	54 (100%)	0	0	100	100
1	U9	54/116 (47%)	54 (100%)	0	0	100	100
1	V1	54/116 (47%)	54 (100%)	0	0	100	100
1	V5	54/116 (47%)	54 (100%)	0	0	100	100
1	V6	54/116 (47%)	54 (100%)	0	0	100	100
1	V9	54/116 (47%)	54 (100%)	0	0	100	100
1	W1	54/116 (47%)	54 (100%)	0	0	100	100
1	W5	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	W6	54/116 (47%)	54 (100%)	0	0	100	100
1	W9	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	X1	54/116 (47%)	54 (100%)	0	0	100	100
1	X5	54/116 (47%)	54 (100%)	0	0	100	100
1	X6	54/116 (47%)	54 (100%)	0	0	100	100
1	X9	54/116 (47%)	54 (100%)	0	0	100	100
1	Y1	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	Y5	54/116 (47%)	54 (100%)	0	0	100	100
1	Y6	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	Y9	54/116 (47%)	54 (100%)	0	0	100	100
1	a3	54/116 (47%)	54 (100%)	0	0	100	100
1	a7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	a8	54/116 (47%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b3	54/116 (47%)	54 (100%)	0	0	100	100
1	b7	54/116 (47%)	54 (100%)	0	0	100	100
1	b8	54/116 (47%)	54 (100%)	0	0	100	100
1	c2	54/116 (47%)	54 (100%)	0	0	100	100
1	c7	54/116 (47%)	54 (100%)	0	0	100	100
1	c8	54/116 (47%)	54 (100%)	0	0	100	100
1	d2	54/116 (47%)	54 (100%)	0	0	100	100
1	d7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	d8	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	e2	54/116 (47%)	54 (100%)	0	0	100	100
1	e7	54/116 (47%)	54 (100%)	0	0	100	100
1	e8	54/116 (47%)	54 (100%)	0	0	100	100
1	f2	54/116 (47%)	54 (100%)	0	0	100	100
1	f7	54/116 (47%)	54 (100%)	0	0	100	100
1	f8	54/116 (47%)	54 (100%)	0	0	100	100
1	g2	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	g7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	g8	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	h2	54/116 (47%)	54 (100%)	0	0	100	100
1	h7	54/116 (47%)	54 (100%)	0	0	100	100
1	h8	54/116 (47%)	54 (100%)	0	0	100	100
1	i3	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	i7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	j3	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	j7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	k3	54/116 (47%)	54 (100%)	0	0	100	100
1	k7	54/116 (47%)	54 (100%)	0	0	100	100
1	l3	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	l7	54/116 (47%)	54 (100%)	0	0	100	100
1	m3	54/116 (47%)	54 (100%)	0	0	100	100
1	m7	54/116 (47%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	m8	54/116 (47%)	54 (100%)	0	0	100	100
1	n3	54/116 (47%)	54 (100%)	0	0	100	100
1	n7	54/116 (47%)	54 (100%)	0	0	100	100
1	n8	54/116 (47%)	54 (100%)	0	0	100	100
1	o3	54/116 (47%)	54 (100%)	0	0	100	100
1	o7	54/116 (47%)	54 (100%)	0	0	100	100
1	o8	54/116 (47%)	54 (100%)	0	0	100	100
1	p3	54/116 (47%)	54 (100%)	0	0	100	100
1	p7	54/116 (47%)	54 (100%)	0	0	100	100
1	p8	54/116 (47%)	54 (100%)	0	0	100	100
1	r3	54/116 (47%)	54 (100%)	0	0	100	100
1	r7	54/116 (47%)	54 (100%)	0	0	100	100
1	s3	54/116 (47%)	54 (100%)	0	0	100	100
1	s7	54/116 (47%)	54 (100%)	0	0	100	100
1	t3	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	t7	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	t8	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	u3	54/116 (47%)	54 (100%)	0	0	100	100
1	u7	54/116 (47%)	54 (100%)	0	0	100	100
1	u8	54/116 (47%)	54 (100%)	0	0	100	100
1	v2	54/116 (47%)	54 (100%)	0	0	100	100
1	v7	54/116 (47%)	54 (100%)	0	0	100	100
1	v8	54/116 (47%)	54 (100%)	0	0	100	100
1	w2	54/116 (47%)	54 (100%)	0	0	100	100
1	w7	54/116 (47%)	54 (100%)	0	0	100	100
1	w8	54/116 (47%)	54 (100%)	0	0	100	100
1	x2	54/116 (47%)	54 (100%)	0	0	100	100
1	x7	54/116 (47%)	54 (100%)	0	0	100	100
1	x8	54/116 (47%)	54 (100%)	0	0	100	100
1	y2	54/116 (47%)	53 (98%)	1 (2%)	0	100	100
1	y7	54/116 (47%)	54 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y8	54/116 (47%)	54 (100%)	0	0	100	100
All	All	8370/17980 (47%)	8329 (100%)	41 (0%)	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	A1	53/103 (52%)	53 (100%)	0	100	100
1	A4	53/103 (52%)	53 (100%)	0	100	100
1	A5	53/103 (52%)	53 (100%)	0	100	100
1	A9	53/103 (52%)	53 (100%)	0	100	100
1	B1	53/103 (52%)	53 (100%)	0	100	100
1	B4	53/103 (52%)	53 (100%)	0	100	100
1	B5	53/103 (52%)	53 (100%)	0	100	100
1	B9	53/103 (52%)	53 (100%)	0	100	100
1	C1	53/103 (52%)	53 (100%)	0	100	100
1	C5	53/103 (52%)	53 (100%)	0	100	100
1	C6	53/103 (52%)	53 (100%)	0	100	100
1	C9	53/103 (52%)	53 (100%)	0	100	100
1	D1	53/103 (52%)	53 (100%)	0	100	100
1	D5	53/103 (52%)	53 (100%)	0	100	100
1	D6	53/103 (52%)	53 (100%)	0	100	100
1	D9	53/103 (52%)	53 (100%)	0	100	100
1	E1	53/103 (52%)	53 (100%)	0	100	100
1	E5	53/103 (52%)	53 (100%)	0	100	100
1	E6	53/103 (52%)	53 (100%)	0	100	100
1	E9	53/103 (52%)	52 (98%)	1 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F1	53/103 (52%)	53 (100%)	0	100	100
1	F5	53/103 (52%)	53 (100%)	0	100	100
1	F6	53/103 (52%)	53 (100%)	0	100	100
1	F9	53/103 (52%)	53 (100%)	0	100	100
1	G1	53/103 (52%)	53 (100%)	0	100	100
1	G5	53/103 (52%)	53 (100%)	0	100	100
1	G6	53/103 (52%)	53 (100%)	0	100	100
1	G9	53/103 (52%)	53 (100%)	0	100	100
1	H1	53/103 (52%)	53 (100%)	0	100	100
1	H5	53/103 (52%)	53 (100%)	0	100	100
1	H6	53/103 (52%)	53 (100%)	0	100	100
1	H9	53/103 (52%)	53 (100%)	0	100	100
1	I1	53/103 (52%)	53 (100%)	0	100	100
1	I4	53/103 (52%)	53 (100%)	0	100	100
1	I9	53/103 (52%)	53 (100%)	0	100	100
1	J1	53/103 (52%)	53 (100%)	0	100	100
1	J4	53/103 (52%)	53 (100%)	0	100	100
1	J9	53/103 (52%)	53 (100%)	0	100	100
1	K1	53/103 (52%)	53 (100%)	0	100	100
1	K4	53/103 (52%)	53 (100%)	0	100	100
1	K9	53/103 (52%)	53 (100%)	0	100	100
1	L1	53/103 (52%)	53 (100%)	0	100	100
1	L4	53/103 (52%)	53 (100%)	0	100	100
1	L9	53/103 (52%)	53 (100%)	0	100	100
1	M1	53/103 (52%)	53 (100%)	0	100	100
1	M4	53/103 (52%)	53 (100%)	0	100	100
1	M5	53/103 (52%)	53 (100%)	0	100	100
1	M9	53/103 (52%)	53 (100%)	0	100	100
1	N1	53/103 (52%)	53 (100%)	0	100	100
1	N4	53/103 (52%)	53 (100%)	0	100	100
1	N5	53/103 (52%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N9	53/103 (52%)	53 (100%)	0	100	100
1	O1	53/103 (52%)	53 (100%)	0	100	100
1	O4	53/103 (52%)	53 (100%)	0	100	100
1	O5	53/103 (52%)	53 (100%)	0	100	100
1	O9	53/103 (52%)	53 (100%)	0	100	100
1	P1	53/103 (52%)	53 (100%)	0	100	100
1	P5	53/103 (52%)	53 (100%)	0	100	100
1	P9	53/103 (52%)	53 (100%)	0	100	100
1	R1	53/103 (52%)	52 (98%)	1 (2%)	50	67
1	R4	53/103 (52%)	53 (100%)	0	100	100
1	R9	53/103 (52%)	53 (100%)	0	100	100
1	S1	53/103 (52%)	53 (100%)	0	100	100
1	S4	53/103 (52%)	53 (100%)	0	100	100
1	S9	53/103 (52%)	53 (100%)	0	100	100
1	T1	53/103 (52%)	53 (100%)	0	100	100
1	T4	53/103 (52%)	53 (100%)	0	100	100
1	T5	53/103 (52%)	53 (100%)	0	100	100
1	T9	53/103 (52%)	53 (100%)	0	100	100
1	U1	53/103 (52%)	53 (100%)	0	100	100
1	U4	53/103 (52%)	53 (100%)	0	100	100
1	U5	53/103 (52%)	53 (100%)	0	100	100
1	U9	53/103 (52%)	53 (100%)	0	100	100
1	V1	53/103 (52%)	53 (100%)	0	100	100
1	V5	53/103 (52%)	53 (100%)	0	100	100
1	V6	53/103 (52%)	52 (98%)	1 (2%)	50	67
1	V9	53/103 (52%)	53 (100%)	0	100	100
1	W1	53/103 (52%)	53 (100%)	0	100	100
1	W5	53/103 (52%)	53 (100%)	0	100	100
1	W6	53/103 (52%)	53 (100%)	0	100	100
1	W9	53/103 (52%)	53 (100%)	0	100	100
1	X1	53/103 (52%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X5	53/103 (52%)	53 (100%)	0	100	100
1	X6	53/103 (52%)	53 (100%)	0	100	100
1	X9	53/103 (52%)	53 (100%)	0	100	100
1	Y1	53/103 (52%)	53 (100%)	0	100	100
1	Y5	53/103 (52%)	53 (100%)	0	100	100
1	Y6	53/103 (52%)	53 (100%)	0	100	100
1	Y9	53/103 (52%)	53 (100%)	0	100	100
1	a3	53/103 (52%)	53 (100%)	0	100	100
1	a7	53/103 (52%)	53 (100%)	0	100	100
1	a8	53/103 (52%)	53 (100%)	0	100	100
1	b3	53/103 (52%)	53 (100%)	0	100	100
1	b7	53/103 (52%)	53 (100%)	0	100	100
1	b8	53/103 (52%)	53 (100%)	0	100	100
1	c2	53/103 (52%)	53 (100%)	0	100	100
1	c7	53/103 (52%)	53 (100%)	0	100	100
1	c8	53/103 (52%)	53 (100%)	0	100	100
1	d2	53/103 (52%)	53 (100%)	0	100	100
1	d7	53/103 (52%)	53 (100%)	0	100	100
1	d8	53/103 (52%)	53 (100%)	0	100	100
1	e2	53/103 (52%)	53 (100%)	0	100	100
1	e7	53/103 (52%)	53 (100%)	0	100	100
1	e8	53/103 (52%)	53 (100%)	0	100	100
1	f2	53/103 (52%)	53 (100%)	0	100	100
1	f7	53/103 (52%)	53 (100%)	0	100	100
1	f8	53/103 (52%)	53 (100%)	0	100	100
1	g2	53/103 (52%)	53 (100%)	0	100	100
1	g7	53/103 (52%)	53 (100%)	0	100	100
1	g8	53/103 (52%)	53 (100%)	0	100	100
1	h2	53/103 (52%)	53 (100%)	0	100	100
1	h7	53/103 (52%)	53 (100%)	0	100	100
1	h8	53/103 (52%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i3	53/103 (52%)	53 (100%)	0	100	100
1	i7	53/103 (52%)	53 (100%)	0	100	100
1	j3	53/103 (52%)	53 (100%)	0	100	100
1	j7	53/103 (52%)	53 (100%)	0	100	100
1	k3	53/103 (52%)	53 (100%)	0	100	100
1	k7	53/103 (52%)	53 (100%)	0	100	100
1	l3	53/103 (52%)	53 (100%)	0	100	100
1	l7	53/103 (52%)	53 (100%)	0	100	100
1	m3	53/103 (52%)	53 (100%)	0	100	100
1	m7	53/103 (52%)	53 (100%)	0	100	100
1	m8	53/103 (52%)	53 (100%)	0	100	100
1	n3	53/103 (52%)	53 (100%)	0	100	100
1	n7	53/103 (52%)	53 (100%)	0	100	100
1	n8	53/103 (52%)	53 (100%)	0	100	100
1	o3	53/103 (52%)	53 (100%)	0	100	100
1	o7	53/103 (52%)	53 (100%)	0	100	100
1	o8	53/103 (52%)	53 (100%)	0	100	100
1	p3	53/103 (52%)	53 (100%)	0	100	100
1	p7	53/103 (52%)	53 (100%)	0	100	100
1	p8	53/103 (52%)	53 (100%)	0	100	100
1	r3	53/103 (52%)	53 (100%)	0	100	100
1	r7	53/103 (52%)	53 (100%)	0	100	100
1	s3	53/103 (52%)	53 (100%)	0	100	100
1	s7	53/103 (52%)	53 (100%)	0	100	100
1	t3	53/103 (52%)	53 (100%)	0	100	100
1	t7	53/103 (52%)	53 (100%)	0	100	100
1	t8	53/103 (52%)	53 (100%)	0	100	100
1	u3	53/103 (52%)	53 (100%)	0	100	100
1	u7	53/103 (52%)	53 (100%)	0	100	100
1	u8	53/103 (52%)	53 (100%)	0	100	100
1	v2	53/103 (52%)	52 (98%)	1 (2%)	50	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v7	53/103 (52%)	53 (100%)	0	100	100
1	v8	53/103 (52%)	53 (100%)	0	100	100
1	w2	53/103 (52%)	53 (100%)	0	100	100
1	w7	53/103 (52%)	53 (100%)	0	100	100
1	w8	53/103 (52%)	53 (100%)	0	100	100
1	x2	53/103 (52%)	53 (100%)	0	100	100
1	x7	53/103 (52%)	53 (100%)	0	100	100
1	x8	53/103 (52%)	53 (100%)	0	100	100
1	y2	53/103 (52%)	53 (100%)	0	100	100
1	y7	53/103 (52%)	53 (100%)	0	100	100
1	y8	53/103 (52%)	53 (100%)	0	100	100
All	All	8215/15965 (52%)	8211 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R1	16	VAL
1	v2	16	VAL
1	V6	16	VAL
1	E9	16	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	26	ASN
1	C1	53	HIS
1	E1	30	ASN
1	G1	53	HIS
1	I1	26	ASN
1	K1	26	ASN
1	K1	53	HIS
1	M1	53	HIS
1	R1	53	HIS
1	U1	53	HIS
1	V1	26	ASN
1	V1	53	HIS
1	X1	30	ASN

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Mol	Chain	Res	Type
1	X1	53	HIS
1	c2	53	HIS
1	e2	30	ASN
1	h2	53	HIS
1	v2	26	ASN
1	v2	53	HIS
1	x2	30	ASN
1	x2	53	HIS
1	i3	26	ASN
1	i3	53	HIS
1	k3	26	ASN
1	m3	53	HIS
1	o3	53	HIS
1	I4	26	ASN
1	K4	26	ASN
1	K4	53	HIS
1	M4	53	HIS
1	A5	26	ASN
1	E5	30	ASN
1	G5	53	HIS
1	H5	53	HIS
1	M5	53	HIS
1	O5	53	HIS
1	V5	53	HIS
1	X5	53	HIS
1	E6	30	ASN
1	H6	53	HIS
1	V6	26	ASN
1	V6	53	HIS
1	X6	30	ASN
1	X6	53	HIS
1	a7	26	ASN
1	a7	53	HIS
1	c7	53	HIS
1	e7	30	ASN
1	e7	53	HIS
1	g7	53	HIS
1	i7	26	ASN
1	k7	26	ASN
1	m7	53	HIS
1	r7	53	HIS
1	v7	53	HIS

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Mol	Chain	Res	Type
1	x7	30	ASN
1	x7	53	HIS
1	a8	26	ASN
1	a8	53	HIS
1	c8	53	HIS
1	h8	53	HIS
1	m8	53	HIS
1	o8	36	GLN
1	o8	53	HIS
1	p8	53	HIS
1	v8	53	HIS
1	x8	30	ASN
1	x8	53	HIS
1	A9	26	ASN
1	A9	53	HIS
1	E9	53	HIS
1	I9	26	ASN
1	K9	26	ASN
1	O9	36	GLN
1	T9	53	HIS
1	X9	30	ASN
1	X9	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

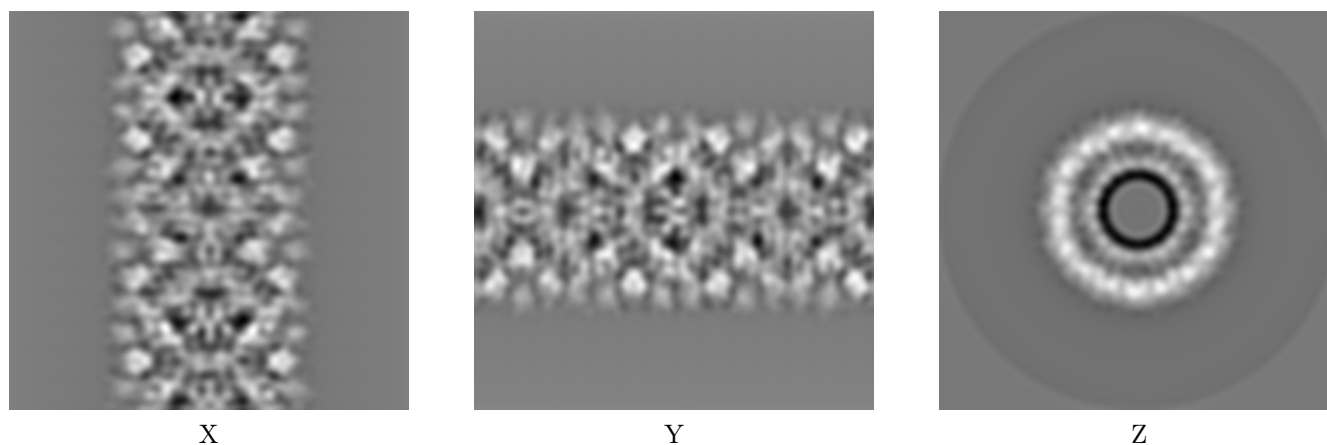
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6439. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

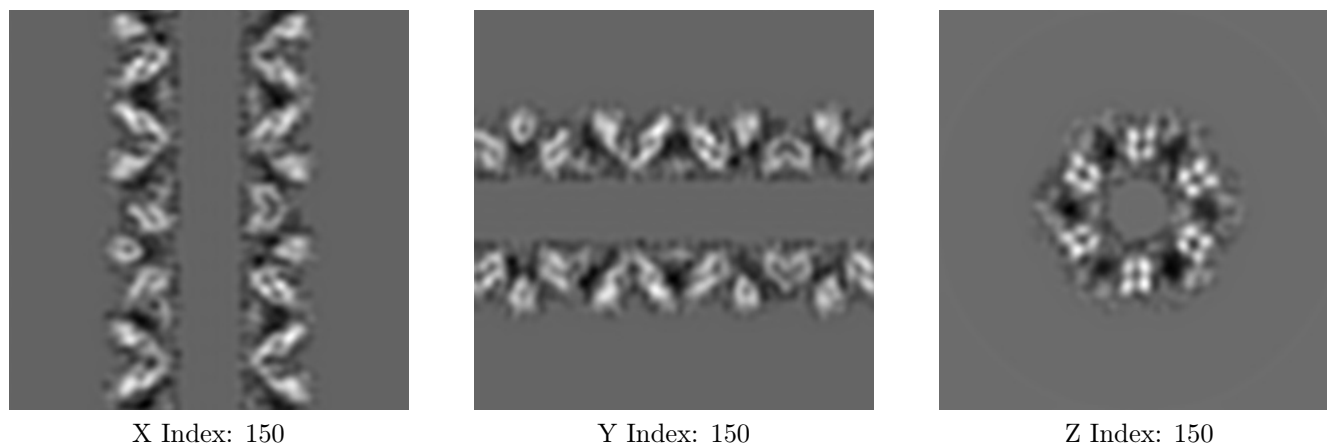
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



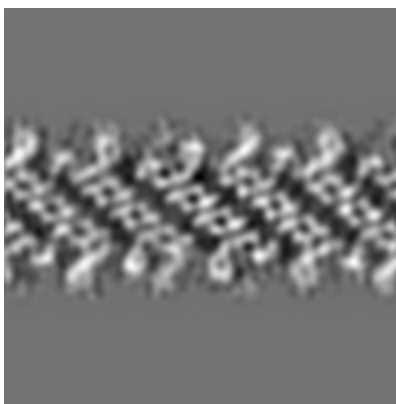
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 189



Y Index: 107

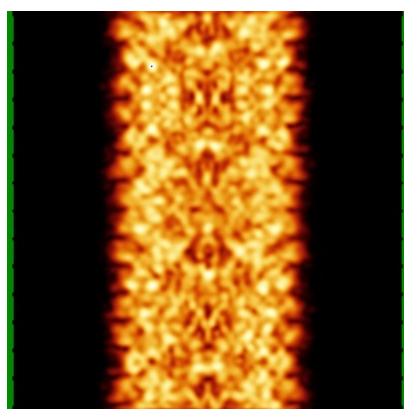


Z Index: 94

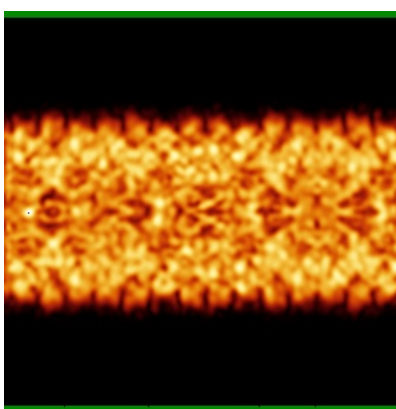
The images above show the largest variance slices of the map in three orthogonal directions.

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

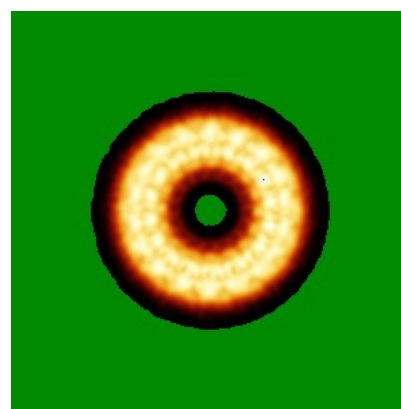
6.4.1 Primary map



X



Y

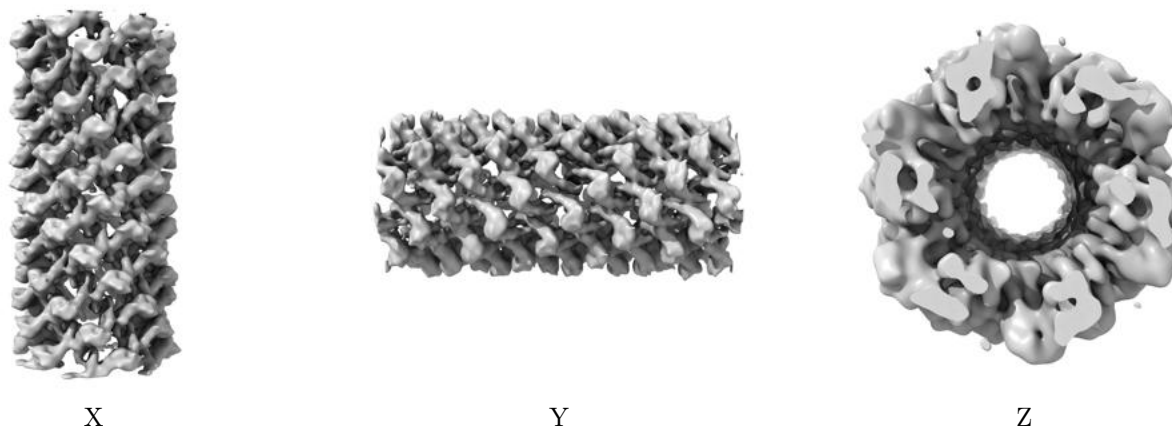


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

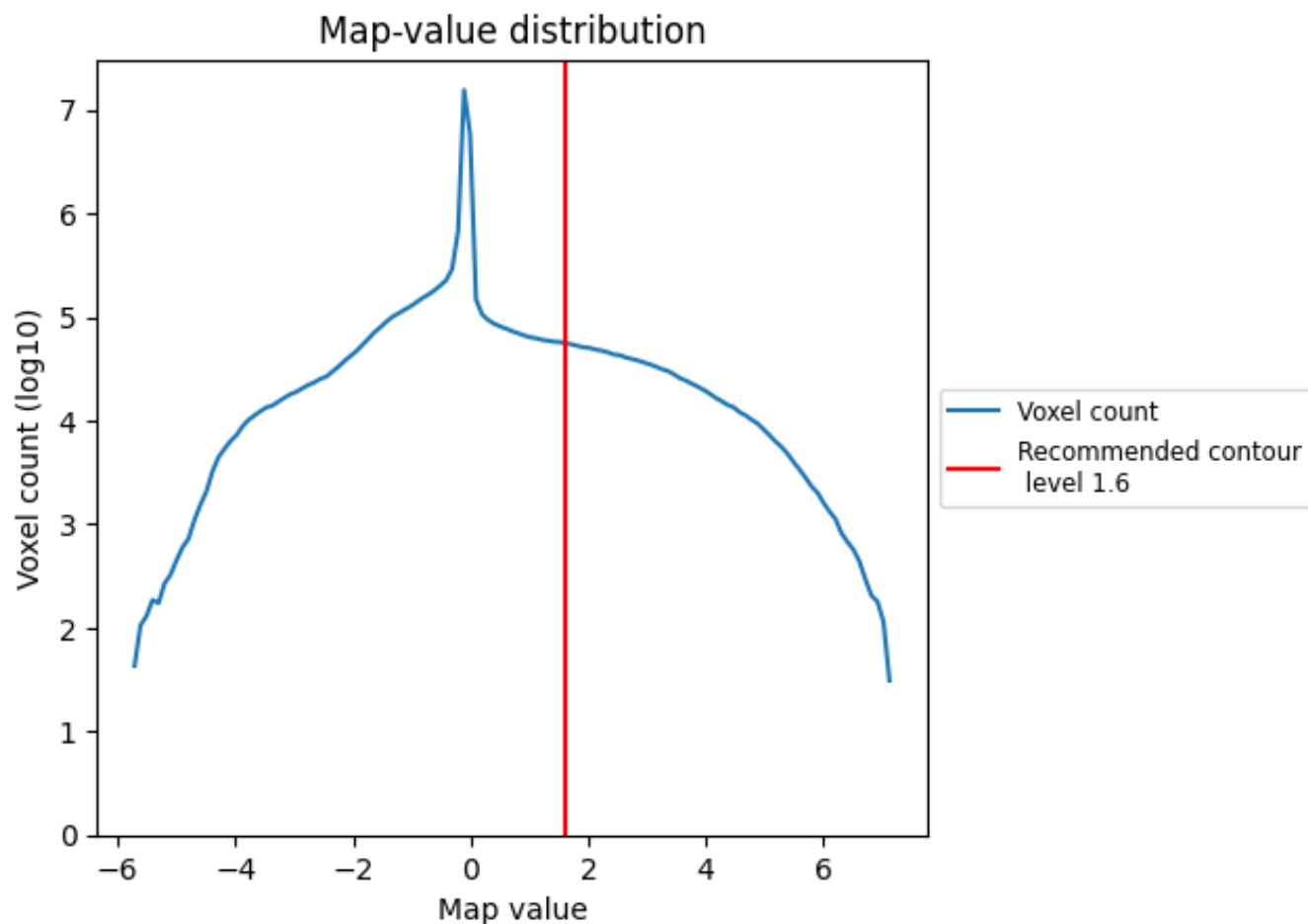
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

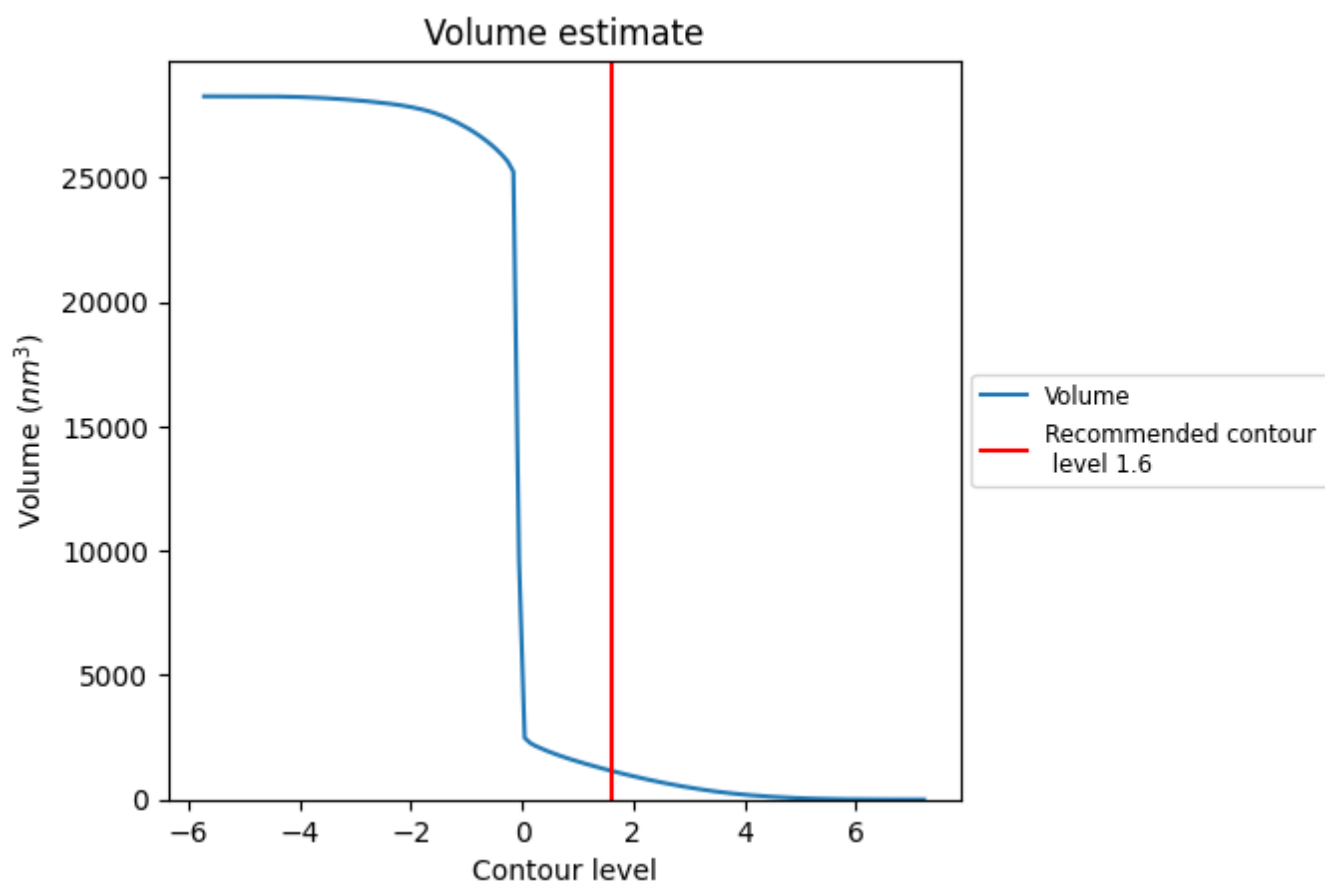
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

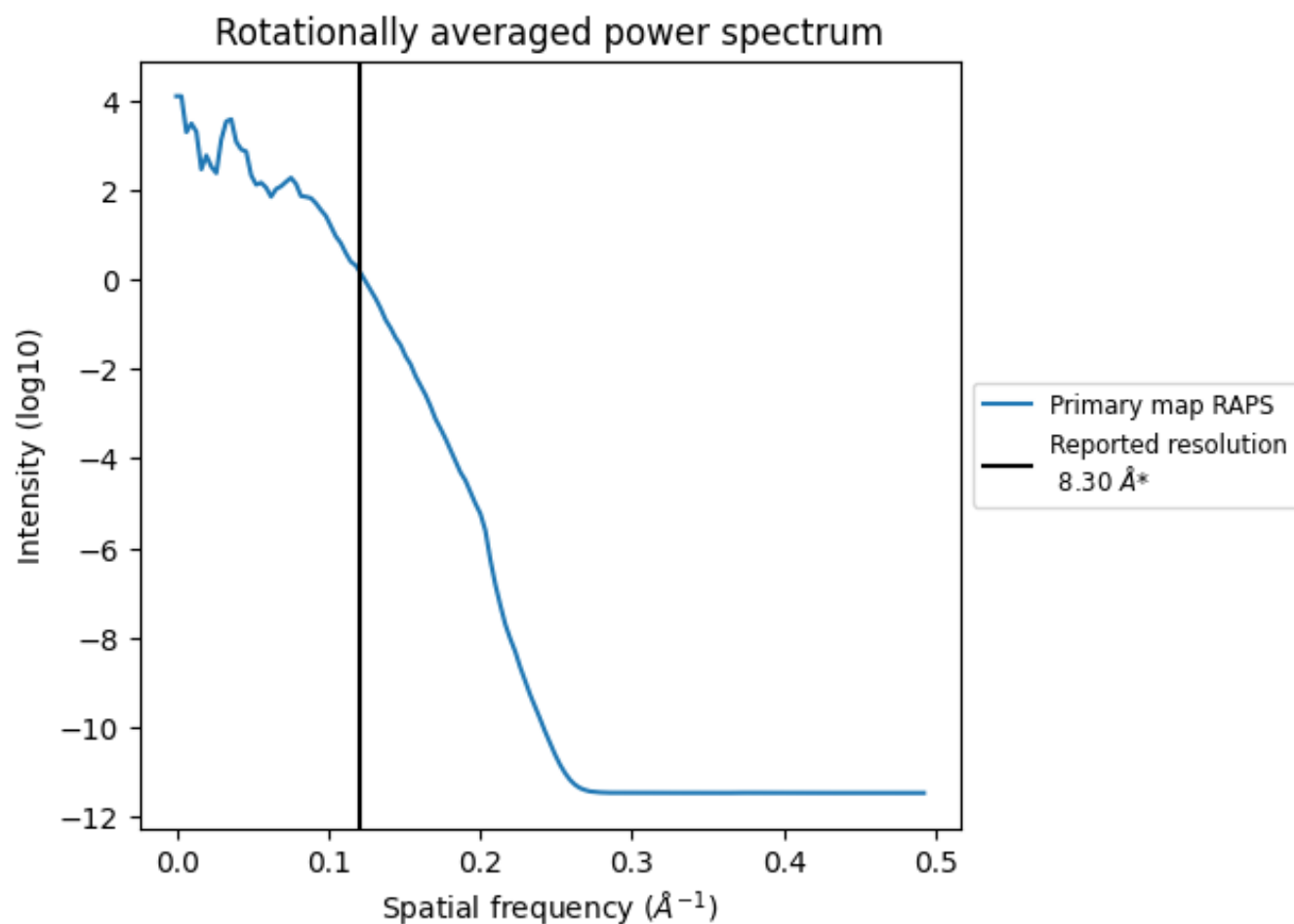
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1159 nm³; this corresponds to an approximate mass of 1047 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 0.120 \AA^{-1}

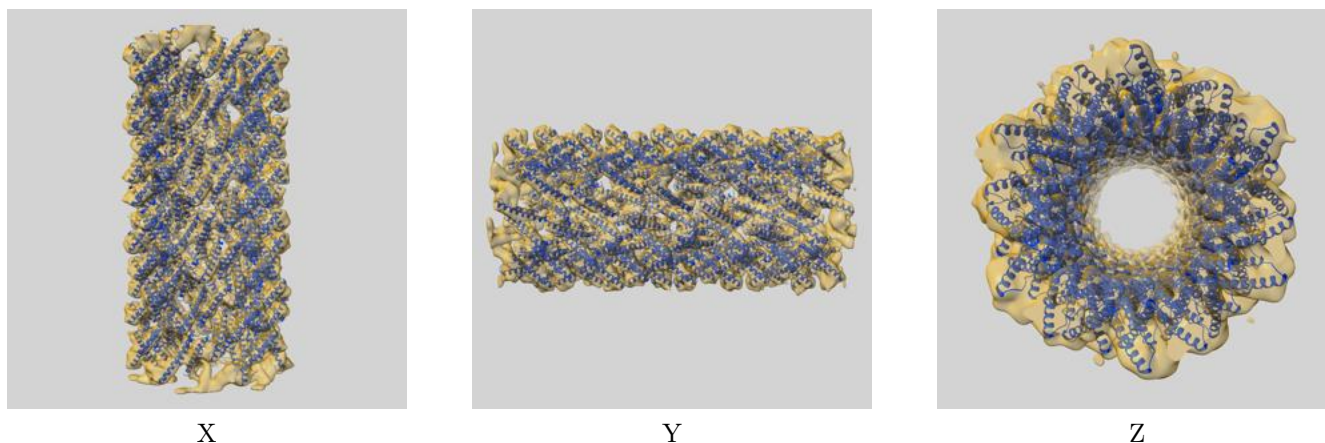
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

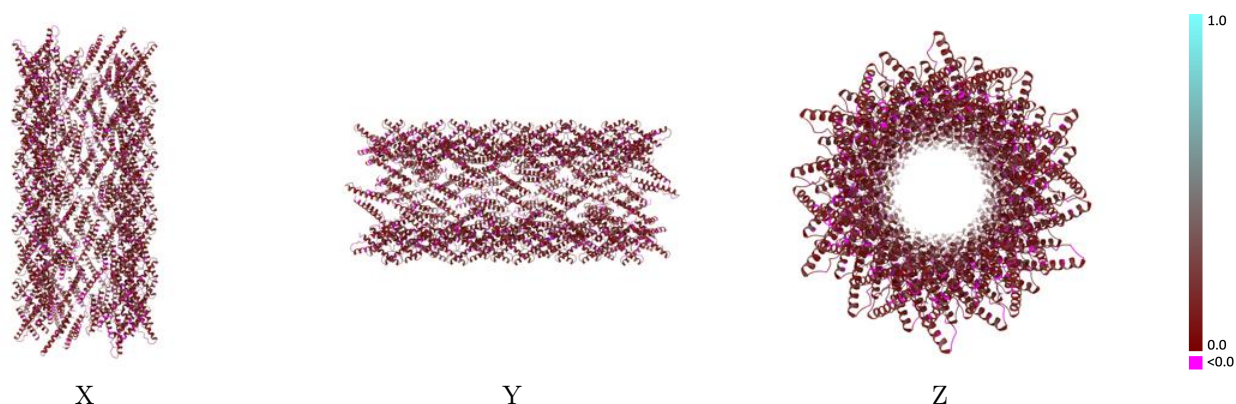
This section contains information regarding the fit between EMDB map EMD-6439 and PDB model 11BE. Per-residue inclusion information can be found in section [3](#) on page [33](#).

9.1 Map-model overlay [i](#)



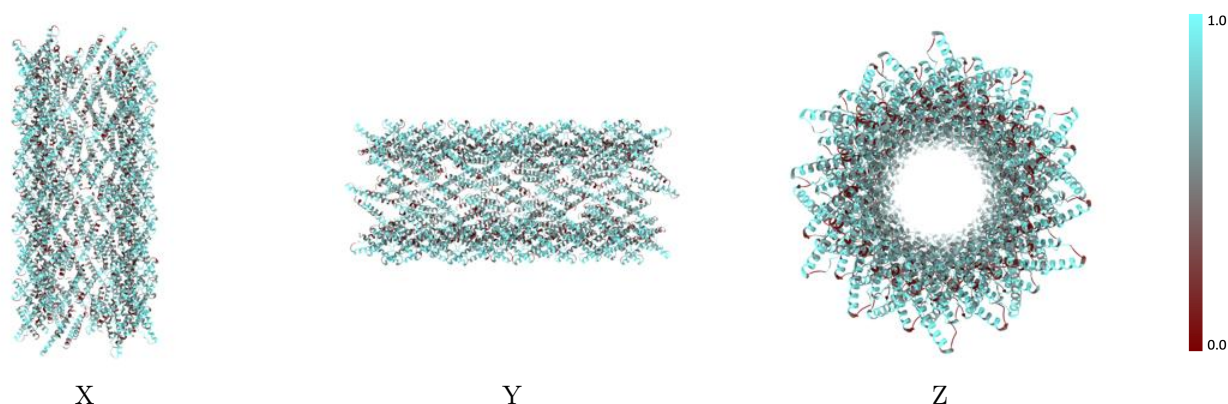
The images above show the 3D surface view of the map at the recommended contour level 1.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



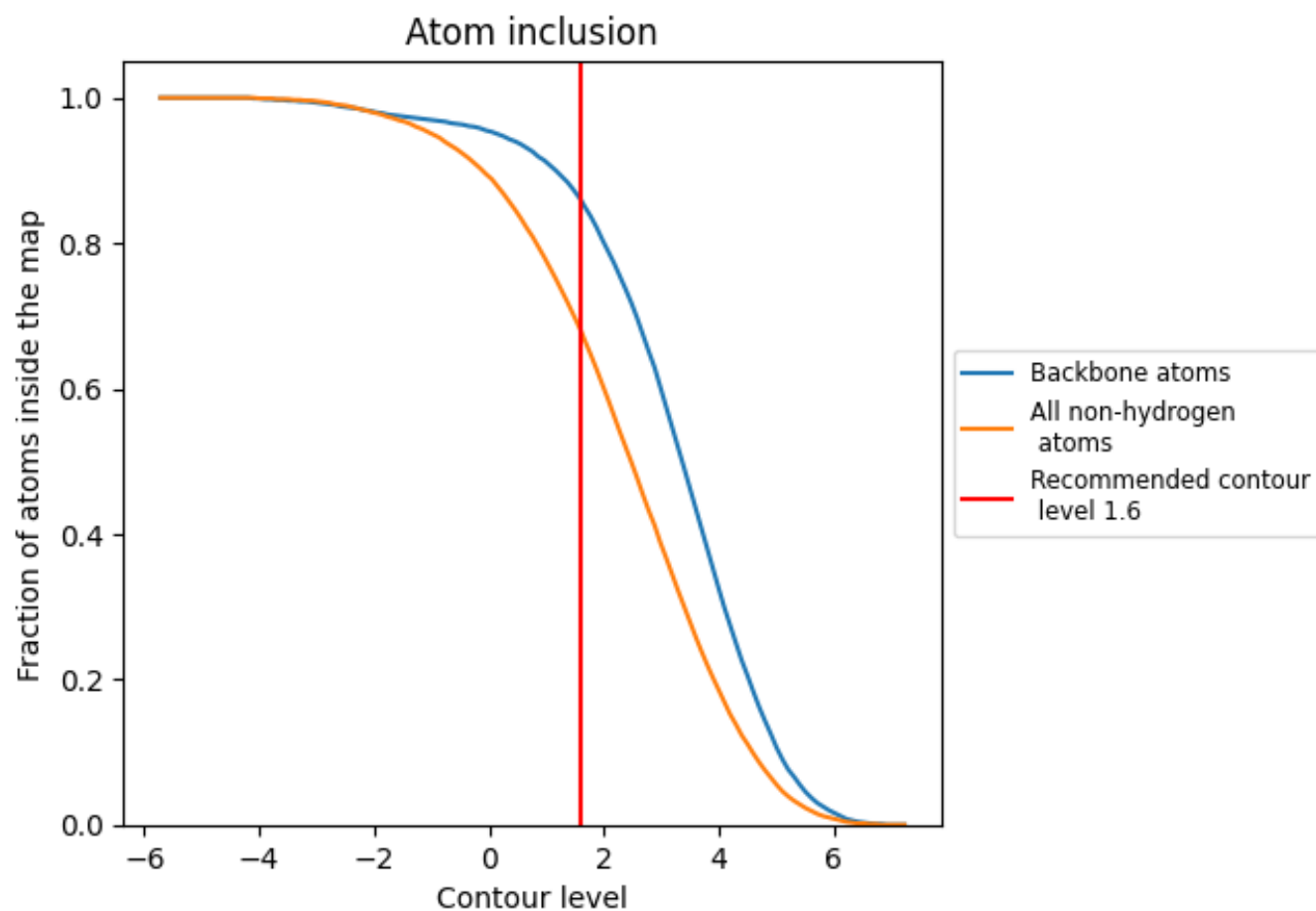
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 68% 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 (1.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6790	 0.1260
A1	 0.6800	 0.1130
A4	 0.6910	 0.1120
A5	 0.6780	 0.1230
A9	 0.6750	 0.1180
B1	 0.7230	 0.1360
B4	 0.7300	 0.1380
B5	 0.6820	 0.1340
B9	 0.6730	 0.1330
C1	 0.6780	 0.1130
C5	 0.6800	 0.1220
C6	 0.6670	 0.1180
C9	 0.6820	 0.1170
D1	 0.7170	 0.1380
D5	 0.6910	 0.1380
D6	 0.6950	 0.1330
D9	 0.6950	 0.1380
E1	 0.6750	 0.1180
E5	 0.6710	 0.1140
E6	 0.6730	 0.1130
E9	 0.6710	 0.1110
F1	 0.7080	 0.1370
F5	 0.6970	 0.1350
F6	 0.7150	 0.1300
F9	 0.6970	 0.1350
G1	 0.6730	 0.1190
G5	 0.6730	 0.1140
G6	 0.6840	 0.1110
G9	 0.6800	 0.1100
H1	 0.6990	 0.1390
H5	 0.6860	 0.1350
H6	 0.6970	 0.1330
H9	 0.6930	 0.1350
I1	 0.6730	 0.1220
I4	 0.6670	 0.1190























































































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Chain	Atom inclusion	Q-score
I9	 0.6780	 0.1140
J1	 0.6840	 0.1350
J4	 0.6930	 0.1350
J9	 0.7100	 0.1370
K1	 0.6750	 0.1180
K4	 0.6670	 0.1180
K9	 0.6890	 0.1120
L1	 0.6890	 0.1340
L4	 0.6890	 0.1340
L9	 0.7230	 0.1350
M1	 0.6580	 0.1210
M4	 0.6510	 0.1170
M5	 0.6600	 0.1170
M9	 0.6640	 0.1170
N1	 0.6670	 0.1360
N4	 0.6580	 0.1350
N5	 0.6970	 0.1370
N9	 0.6820	 0.1350
O1	 0.6580	 0.1250
O4	 0.6450	 0.1150
O5	 0.6750	 0.1210
O9	 0.6750	 0.1200
P1	 0.6600	 0.1340
P5	 0.6800	 0.1340
P9	 0.6820	 0.1310
R1	 0.6730	 0.1100
R4	 0.6640	 0.1060
R9	 0.6690	 0.1110
S1	 0.6990	 0.1370
S4	 0.7020	 0.1330
S9	 0.7060	 0.1370
T1	 0.6820	 0.1090
T4	 0.6670	 0.1110
T5	 0.6820	 0.1140
T9	 0.6780	 0.1150
U1	 0.6890	 0.1360
U4	 0.6990	 0.1310
U5	 0.7320	 0.1380
U9	 0.7100	 0.1380
V1	 0.6360	 0.1080
V5	 0.6470	 0.1200
V6	 0.6430	 0.1180











































































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Chain	Atom inclusion	Q-score
V9	 0.6380	 0.1260
W1	 0.6890	 0.1400
W5	 0.6990	 0.1440
W6	 0.6910	 0.1440
W9	 0.6990	 0.1410
X1	 0.6360	 0.1080
X5	 0.6320	 0.1170
X6	 0.6190	 0.1180
X9	 0.6340	 0.1210
Y1	 0.7040	 0.1380
Y5	 0.6890	 0.1420
Y6	 0.6890	 0.1420
Y9	 0.6930	 0.1360
a3	 0.6380	 0.1110
a7	 0.6360	 0.1050
a8	 0.6380	 0.1020
b3	 0.6840	 0.1440
b7	 0.6990	 0.1400
b8	 0.6970	 0.1420
c2	 0.6450	 0.1020
c7	 0.6320	 0.1060
c8	 0.6380	 0.1060
d2	 0.7100	 0.1350
d7	 0.6930	 0.1440
d8	 0.7040	 0.1420
e2	 0.6640	 0.1210
e7	 0.6690	 0.1170
e8	 0.6580	 0.1230
f2	 0.6950	 0.1240
f7	 0.6690	 0.1310
f8	 0.6670	 0.1270
g2	 0.6820	 0.1270
g7	 0.6730	 0.1220
g8	 0.6800	 0.1240
h2	 0.6730	 0.1250
h7	 0.6750	 0.1320
h8	 0.6800	 0.1330
i3	 0.6450	 0.1080
i7	 0.6450	 0.1190
j3	 0.6890	 0.1370
j7	 0.6860	 0.1400
k3	 0.6400	 0.1090

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Chain	Atom inclusion	Q-score
k7	 0.6360	 0.1220
l3	 0.6950	 0.1360
l7	 0.6840	 0.1370
m3	 0.6640	 0.1200
m7	 0.6450	 0.1140
m8	 0.6400	 0.1130
n3	 0.6970	 0.1290
n7	 0.6620	 0.1350
n8	 0.6890	 0.1370
o3	 0.6820	 0.1120
o7	 0.6430	 0.1170
o8	 0.6450	 0.1140
p3	 0.6970	 0.1310
p7	 0.6730	 0.1320
p8	 0.6710	 0.1330
r3	 0.6780	 0.1180
r7	 0.6780	 0.1240
s3	 0.6730	 0.1270
s7	 0.6970	 0.1370
t3	 0.6750	 0.1260
t7	 0.6820	 0.1260
t8	 0.6730	 0.1210
u3	 0.6780	 0.1280
u7	 0.7190	 0.1390
u8	 0.7170	 0.1370
v2	 0.6690	 0.1130
v7	 0.6670	 0.1100
v8	 0.6690	 0.1100
w2	 0.7190	 0.1390
w7	 0.7280	 0.1320
w8	 0.7260	 0.1390
x2	 0.6690	 0.1070
x7	 0.6640	 0.1090
x8	 0.6710	 0.1100
y2	 0.7150	 0.1380
y7	 0.7170	 0.1370
y8	 0.7150	 0.1380