



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:10 PM UTC

PDB ID : 6RWX / pdb_00006rwx
EMDB ID : EMD-10045
Title : Periplasmic inner membrane ring of the Shigella type 3 secretion system
Authors : Kamprad, A.; Lunelli, M.
Deposited on : 2019-06-06
Resolution : 3.55 Å(reported)
Based on initial models : 3GR0, 2Y9J

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

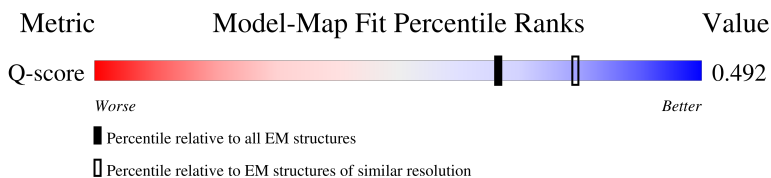
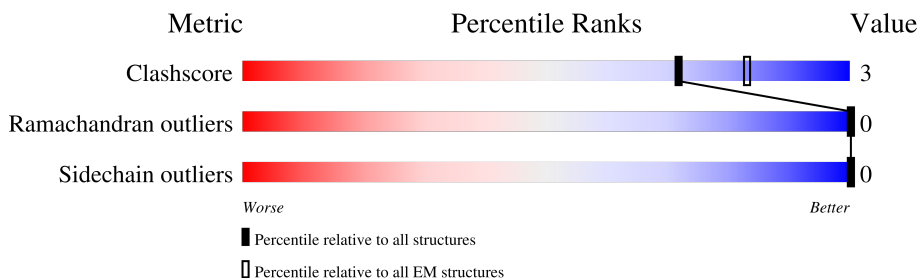
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.55 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.



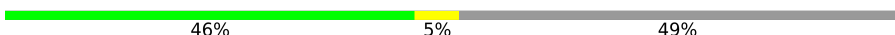
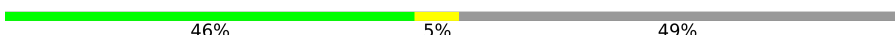
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12819 (3.05 - 4.05)

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

Mol	Chain	Length	Quality of chain
1	A	371	 47% . 49%
1	B	371	 47% . 49%
1	C	371	 48% . 49%
1	D	371	 48% . 49%

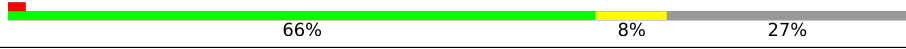
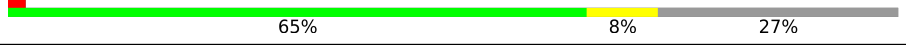
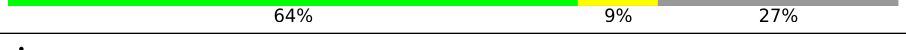
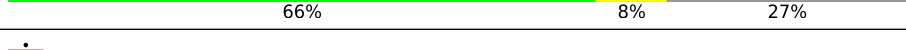
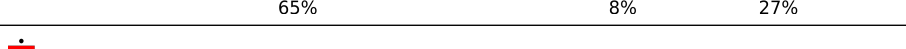
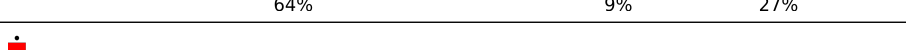
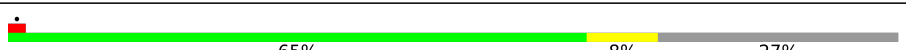
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Mol	Chain	Length	Quality of chain
1	E	371	
1	F	371	
1	G	371	
1	H	371	
1	I	371	
1	J	371	
1	K	371	
1	L	371	
1	M	371	
1	N	371	
1	O	371	
1	P	371	
1	Q	371	
1	R	371	
1	S	371	
1	T	371	
1	U	371	
1	V	371	
1	W	371	
1	X	371	
2	a	241	
2	b	241	
2	c	241	
2	d	241	
2	e	241	

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Mol	Chain	Length	Quality of chain
2	f	241	
2	g	241	
2	h	241	
2	i	241	
2	j	241	
2	k	241	
2	l	241	
2	m	241	
2	n	241	
2	o	241	
2	p	241	
2	q	241	
2	r	241	
2	s	241	
2	t	241	
2	u	241	
2	v	241	
2	w	241	
2	x	241	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 70968 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 MxiG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	T	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	R	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	Q	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	P	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	O	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	N	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	M	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	L	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	K	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	J	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	I	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	H	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	G	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	F	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	E	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	D	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	B	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	A	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	W	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	V	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	U	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		
1	X	189	Total	C	N	O	S	0	0
			1554	994	261	296	3		

- Molecule 2 is a protein called Lipoprotein MxiJ.

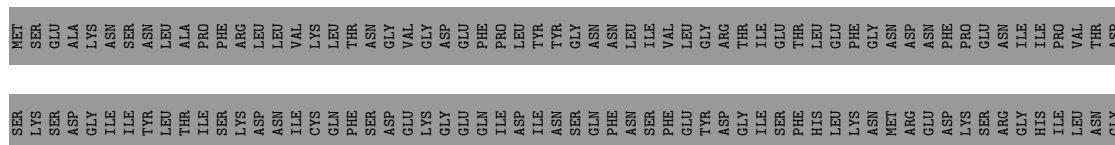
Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	b	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	c	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	d	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	e	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	f	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	g	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	h	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	i	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	j	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	k	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		
2	l	177	Total	C	N	O	S	0	0
			1403	882	241	276	4		

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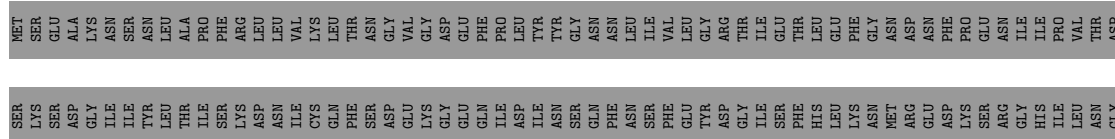
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	m	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	n	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	o	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	p	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	q	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	r	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	s	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	t	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	u	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	v	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	w	177	Total 1403	C 882	N 241	O 276	S 4	0	0
2	x	177	Total 1403	C 882	N 241	O 276	S 4	0	0

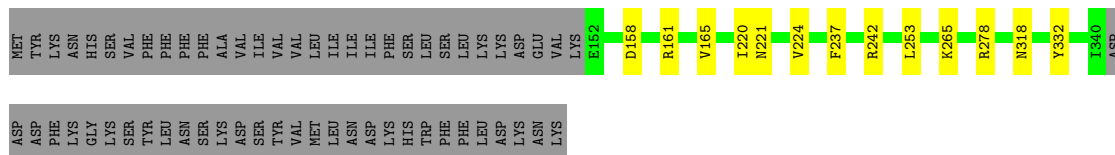
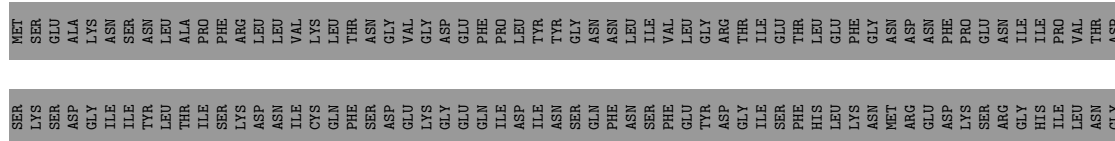
- Molecule 1: Protein MxiG



- Molecule 1: Protein MxiG



- Molecule 1: Protein MxiG



MET	SER	GLU	ALA	LYS	ASN	SER	ASN	LEU	ALA	PRO	PHE	ARG	LEU	LEU	VAL	LYS	LEU	THR	ASN	GLY	VAL	GLY	ASP	ASP	GLU	PHE	PRO	LEU	TYR	TYR	GLY	ASN	ASN	GLY	GLY	LEU	ILE	VAL	VAL	LEU	LEU	GLU	PHE	PHE	GLY	ASN	ASP	ASN	PHE	PRO	GLU	ASN	ILE	ILE	PRO	VAL	THR
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SER	LYS	ASP	GLY	ILE	TYR	LEU	THR	ILE	SER	LYS	ASP	LYS	ASP	GLN	GLY	ASP	GLN	PHE	ASN	SER	PHE	GLY	TYR	ASP	GLY	ILE	SER	PHE	GLN	ILE	ASP	ASN	ILE	ASN	VAL	LYS	ILE	E152												
MET	TYR	LYS	ASN	HIS	SER	VAL	PHE	LEU	PHE	ASN	ALA	VAL	VAL	LEU	ILE	ILE	ILE	PHE	ASP	GLY	SER	LEU	LYS	TRP	HIS	ASP	GLY	ASP	ASP	GLY	ASP	VAL	LYS	D158	R161	V165	I220	N221	V224	F237	R242	L253	K265	R278	N318	Y332	I340	ASP		
ASP	ASP	PHE	LYS	GLY	LYS	SER	TYR	LEU	ASN	SER	LYS	ASP	VAL	VAL	MET	LEU	GLN	ASN	ASP	LYS	GLY	ASP	GLY	TRP	PHE	LEU	ASP	LYS	ASN	VAL	LYS	GLY	ASN	LYS	E152	D158	R161	V165	I220	N221	V224	F237	R242	L253	K265	R278	N318	Y332	I340	ASP

● Molecule 1: Protein MxiG

Chain J:  47% . 49%

I340	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP
	ASP	ASP	ASP	PHE	GLY	LYS	LYS	SER	TYR	ALA	PRO	ILE	SER	ARG	LEU	VAL	VAL	LYS	THR	ILE	ASP	GLY	GLY	TRP	PHE	PRO	LEU	TYR	GLY	ASN	GLY	ASN	PHE	ASN	GLN	PHE	ASN	GLY	ASP	GLY	THR	VAL	THR	ASP

● Molecule 1: Protein MxiG

Chain I:  47% . 49%

ASP	ASP	PHE	LYS	GLY	LYS	SER	TYR	LEU	ASN	SER	LYS	VAL	ASP	ASP	TYR	VAL	VAL	VAL	LEU	ILE	ILE	ILE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
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● Molecule 1: Protein MxiG

Chain H:  47% . 49%

ASP	ASP	PHE	LYS	GLY	LYS	TYR	LEU	ASN	SER	VAL	PHE	PHE	PHE	ALA	VAL	ASP	SER	TYR	VAL	VAL	LEU	ILE	ASN	ASP	PHE	TRP	PHE	PHE	LYS	HIS	LYS	ASN	ASN	LYS	LYS	ASP	ASP	LYS	ASN	ASN	LYS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
MET	TYR	LYS	ASN	HIS	SER	VAL	PHE	PHE	PHE	ALA	VAL	VAL	ILE	ASN	ASP	ILE	PHE	SER	LEU	LEU	ILE	ILE	ILE	GLY	GLY	ASP	GLY	VAL	VAL	LYS	LYS	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE

Chain G:

47%

49%

Sequence logo for Chain G showing amino acid conservation across 47% and 49% of the sequences. The y-axis lists amino acids (MET, SER, LYS, ASN, ASP, PHE, THR, VAL, LEU, THR, GLY, ASP, PHE, VAL, THR, TTR, GLY, ASN, ASN, ASN, ILE, VAL, GLU, LEU, THR, THR, GLU, THR, LEU, GLU, PHE, GLY, ASN, ASP, ASN, PHE, PHE, THR, GLU, ASN, ILE, THR, VAL, THR, ASN, GLY) and the x-axis shows positions 1 to 200. A green bar at the top indicates 47% conservation, and a grey bar indicates 49% conservation. A dot is present at position 100.

[illegible]

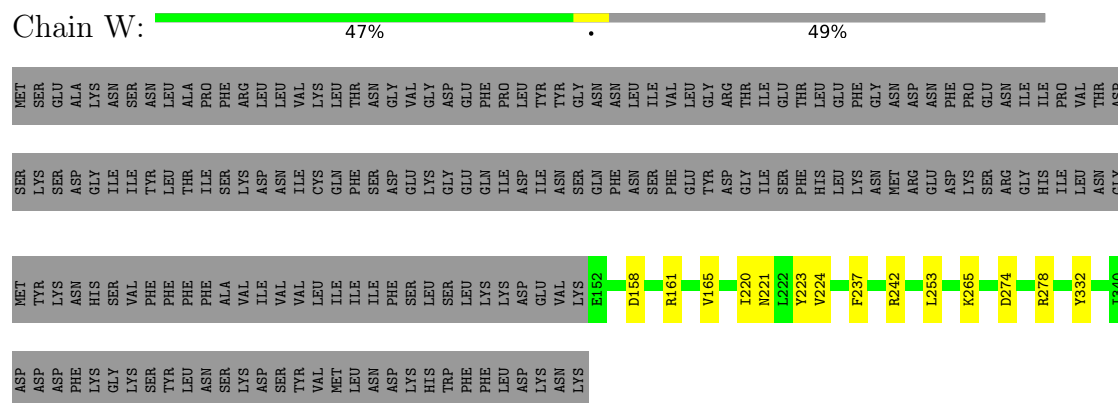
Chain E:

Residue	Information Content (bits)
MET	0.152
TYR	0.158
ASP	0.161
ASP	0.165
ASP	0.182
PHE	0.187
LYS	0.220
GLY	0.221
VAL	0.224
THR	0.237
ASP	0.242
LYS	0.253
ASP	0.265
THR	0.278
ASP	0.332

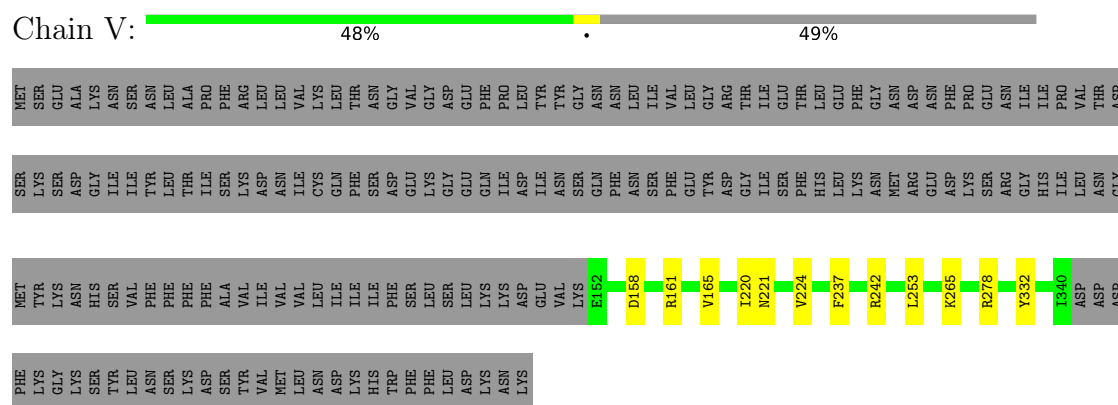
Chain D: 48% 49%

Residue	Green (%)	Grey (%)
MET	0	0
SER	0	0
GLU	0	0
ALA	0	0
LYS	0	0
ASN	0	0
SER	0	0
ASN	0	0
LEU	0	0
ALA	0	0
PRO	0	0
PHE	0	0
ARG	0	0
LEU	0	0
VAL	0	0
LYS	0	0
LEU	0	0
THR	0	0
ASN	0	0
GLY	0	0
VAL	0	0
GLY	0	0
ASP	0	0
GLU	0	0
PHE	0	0
PRO	0	0
LEU	0	0
TYR	0	0
TYR	0	0
GLY	0	0
ASN	0	0
ASN	0	0
LEU	0	0
ILE	0	0
VAL	0	0
LEU	0	0
GLY	0	0
ARG	0	0
THR	0	0
ILE	0	0
GLU	0	0
THR	0	0
LEU	0	0
GLU	0	0
PHE	0	0
GLY	0	0
ASN	0	0
ASP	0	0
ASN	0	0
PHE	0	0
PRO	0	0
GLU	0	0
ASN	0	0
ILE	0	0
ILE	0	0
PRO	0	0
VAL	0	0
THR	0	0
ASP	0	0

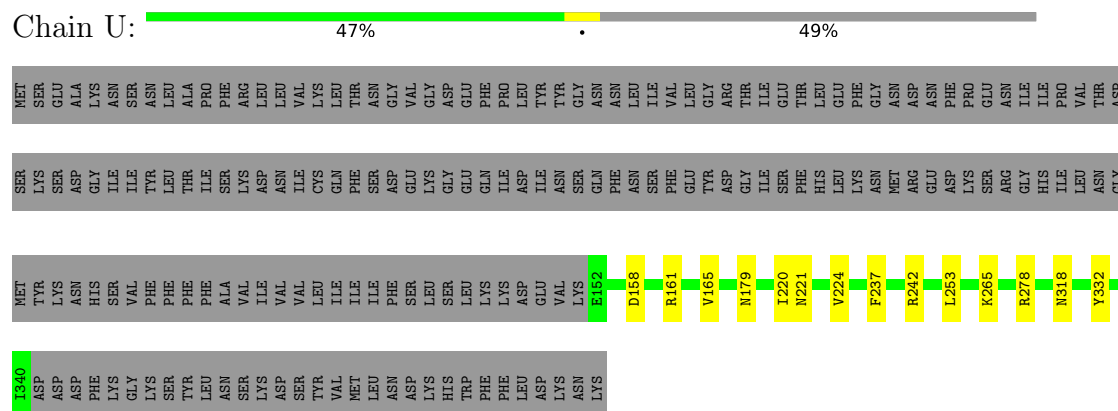
- Molecule 1: Protein MxiG



- Molecule 1: Protein MxiG

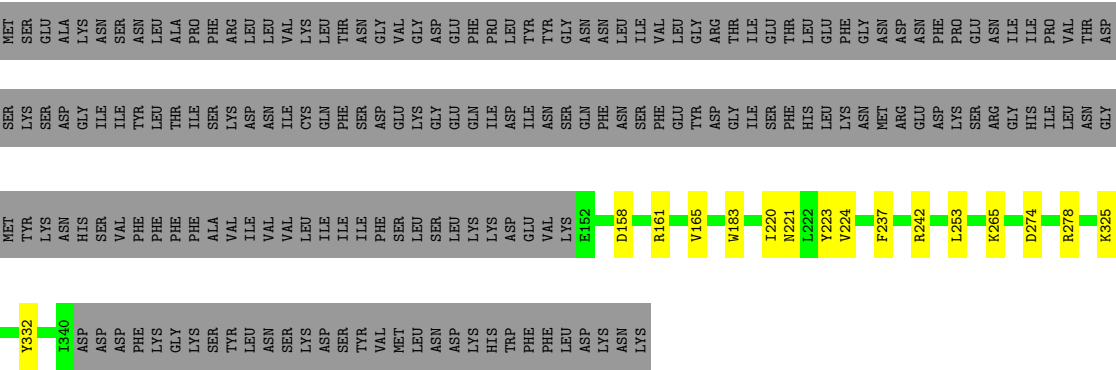


- Molecule 1: Protein MxiG

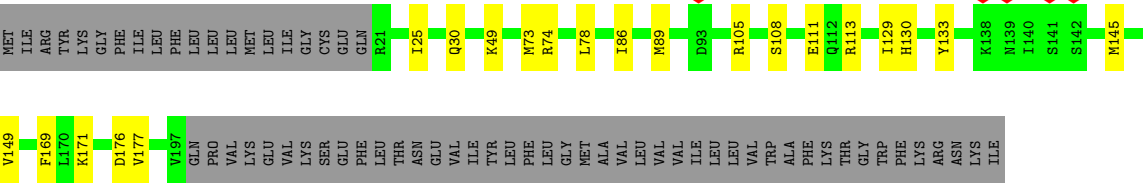


- Molecule 1: Protein MxiG

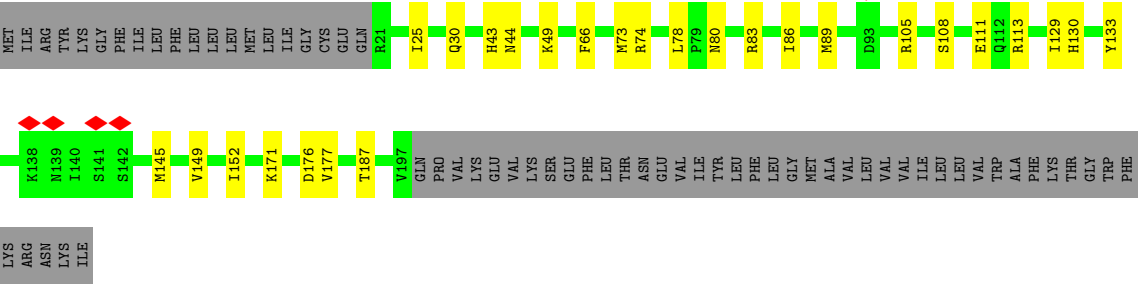




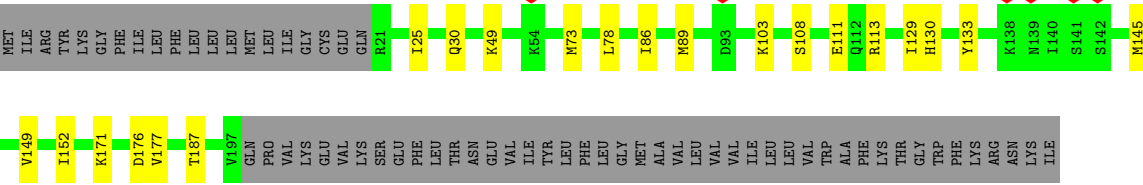
• Molecule 2: Lipoprotein MxiJ



• Molecule 2: Lipoprotein MxiJ



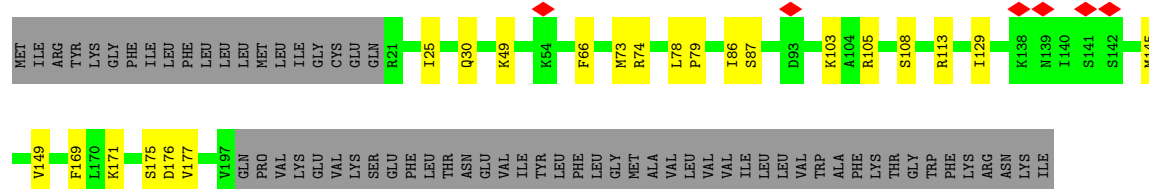
• Molecule 2: Lipoprotein MxiJ



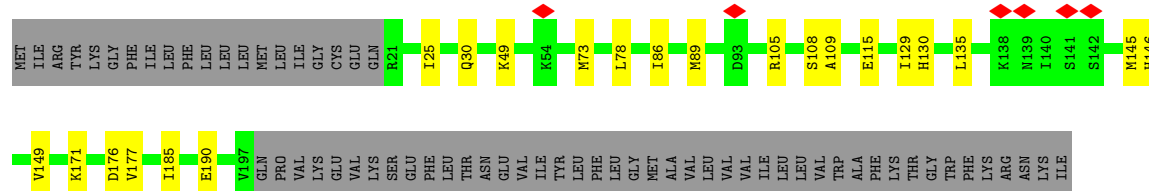
• Molecule 2: Lipoprotein MxiJ



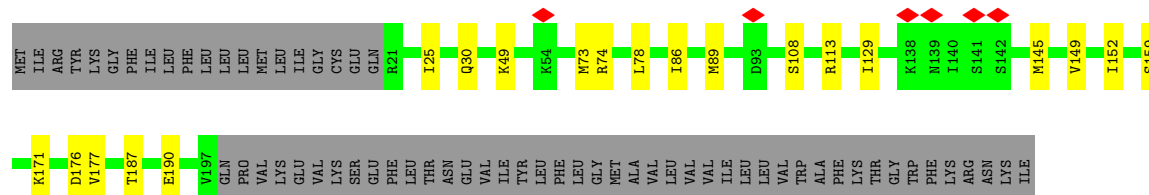
- Molecule 2: Lipoprotein MxiJ



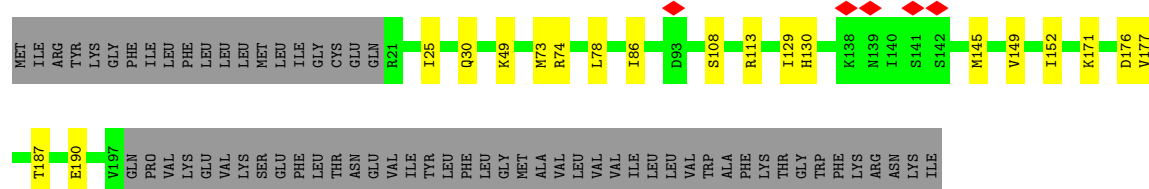
- Molecule 2: Lipoprotein MxiJ



- Molecule 2: Lipoprotein MxiJ

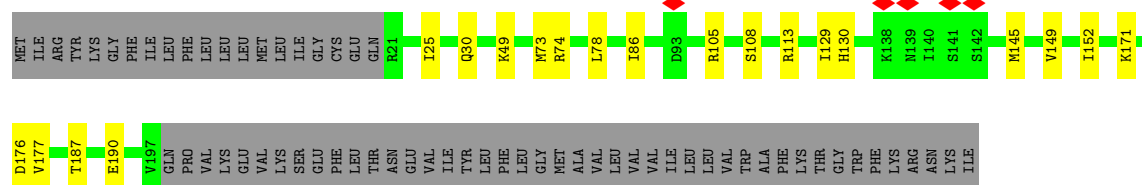


- Molecule 2: Lipoprotein MxiJ



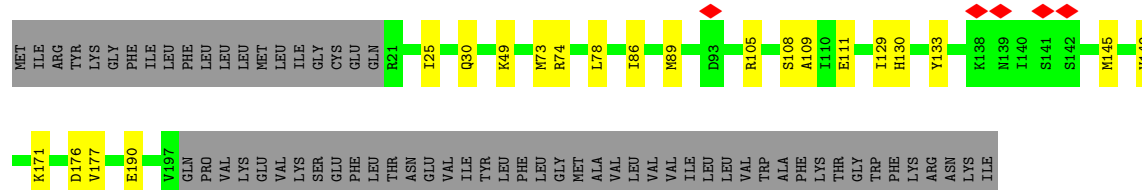
- Molecule 2: Lipoprotein MxiJ

Chain i: 



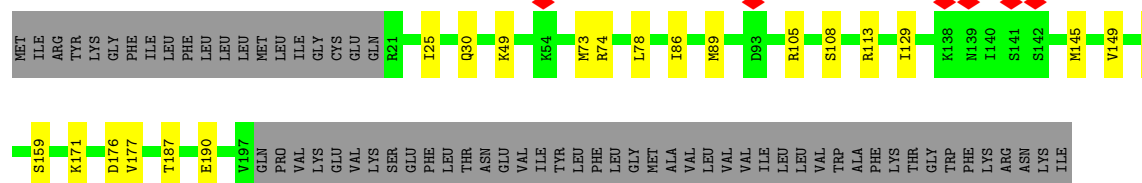
- Molecule 2: Lipoprotein MxiJ

Chain j: 



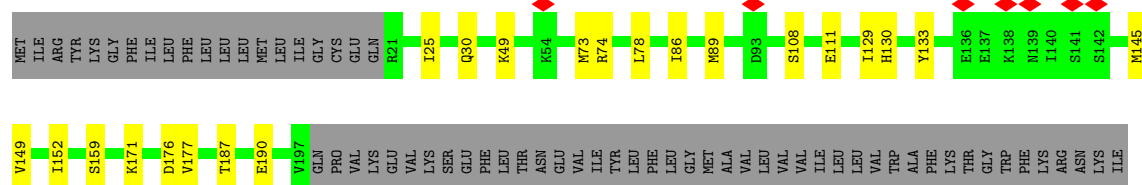
- Molecule 2: Lipoprotein MxiJ

Chain k: 



- Molecule 2: Lipoprotein MxiJ

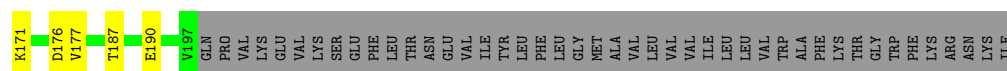
Chain l: 



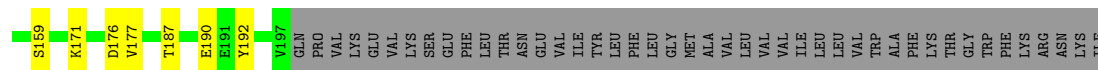
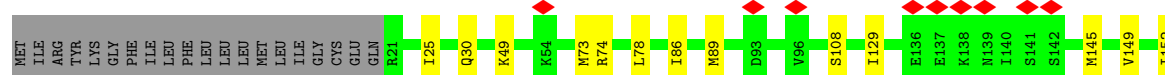
- Molecule 2: Lipoprotein MxiJ

Chain m: 

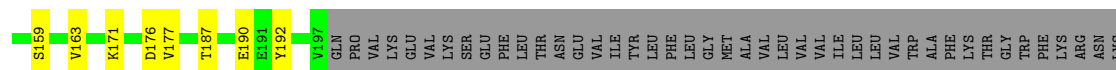




- Molecule 2: Lipoprotein MxiJ

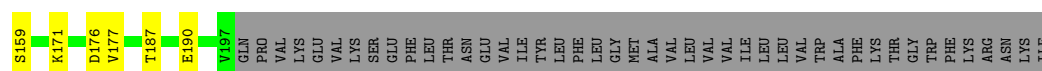


- Molecule 2: Lipoprotein MxiJ

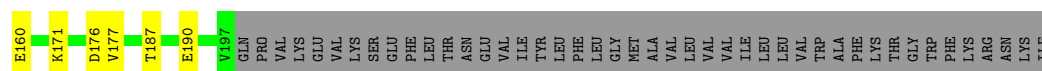
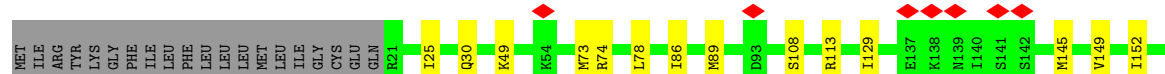


ILE

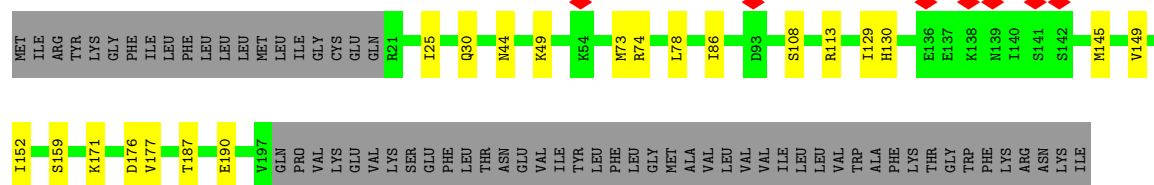
- Molecule 2: Lipoprotein MxiJ



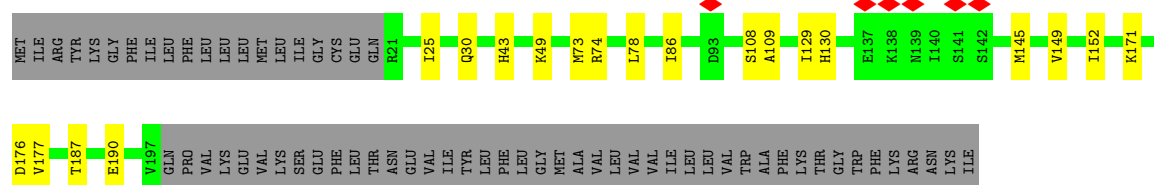
- Molecule 2: Lipoprotein MxiJ



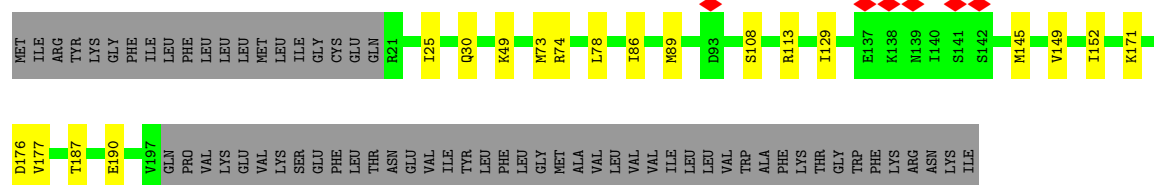
- Molecule 2: Lipoprotein MxiJ



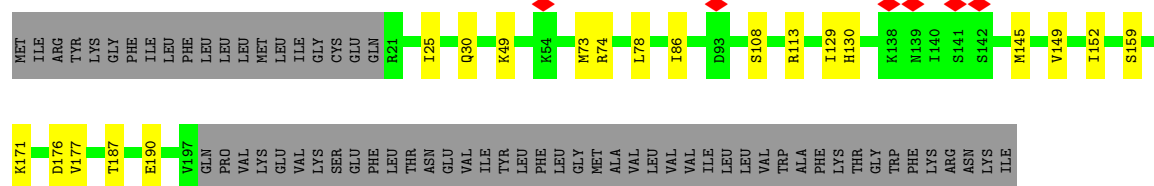
- Molecule 2: Lipoprotein MxiJ



- Molecule 2: Lipoprotein MxiJ

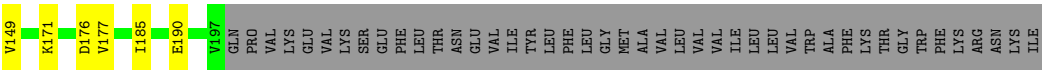


- Molecule 2: Lipoprotein MxiJ

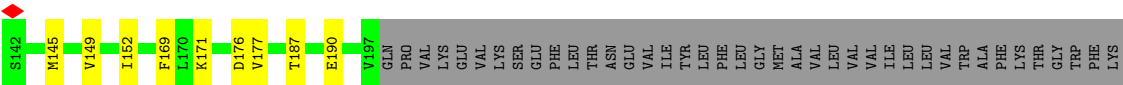


- Molecule 2: Lipoprotein MxiJ





• Molecule 2: Lipoprotein MxiJ



• Molecule 2: Lipoprotein MxiJ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C24	Depositor
Number of particles used	72298	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	4	Depositor
Magnification	101179	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.635	Depositor
Minimum map value	-0.387	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	664.1712, 664.1712, 664.1712	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38369, 1.38369, 1.38369	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	A	0.34	0/1578	0.52	1/2130 (0.0%)
1	B	0.34	0/1578	0.52	1/2130 (0.0%)
1	C	0.34	0/1578	0.52	1/2130 (0.0%)
1	D	0.34	0/1578	0.52	1/2130 (0.0%)
1	E	0.35	0/1578	0.52	1/2130 (0.0%)
1	F	0.35	0/1578	0.52	1/2130 (0.0%)
1	G	0.34	0/1578	0.52	1/2130 (0.0%)
1	H	0.35	0/1578	0.52	1/2130 (0.0%)
1	I	0.35	0/1578	0.52	1/2130 (0.0%)
1	J	0.35	0/1578	0.52	1/2130 (0.0%)
1	K	0.35	0/1578	0.52	1/2130 (0.0%)
1	L	0.34	0/1578	0.52	1/2130 (0.0%)
1	M	0.34	0/1578	0.52	1/2130 (0.0%)
1	N	0.34	0/1578	0.52	1/2130 (0.0%)
1	O	0.34	0/1578	0.52	1/2130 (0.0%)
1	P	0.35	0/1578	0.52	1/2130 (0.0%)
1	Q	0.34	0/1578	0.52	1/2130 (0.0%)
1	R	0.34	0/1578	0.52	1/2130 (0.0%)
1	S	0.34	0/1578	0.52	1/2130 (0.0%)
1	T	0.34	0/1578	0.52	1/2130 (0.0%)
1	U	0.34	0/1578	0.52	1/2130 (0.0%)
1	V	0.34	0/1578	0.52	1/2130 (0.0%)
1	W	0.35	0/1578	0.52	1/2130 (0.0%)
1	X	0.34	0/1578	0.52	1/2130 (0.0%)
2	a	0.37	0/1423	0.55	0/1921
2	b	0.37	0/1423	0.55	0/1921
2	c	0.37	0/1423	0.55	0/1921
2	d	0.37	0/1423	0.55	0/1921
2	e	0.37	0/1423	0.55	0/1921
2	f	0.37	0/1423	0.55	0/1921
2	g	0.37	0/1423	0.55	0/1921
2	h	0.37	0/1423	0.55	0/1921
2	i	0.37	0/1423	0.55	0/1921
2	j	0.37	0/1423	0.55	0/1921

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	k	0.37	0/1423	0.55	0/1921
2	l	0.37	0/1423	0.55	0/1921
2	m	0.37	0/1423	0.55	0/1921
2	n	0.37	0/1423	0.55	0/1921
2	o	0.37	0/1423	0.55	0/1921
2	p	0.37	0/1423	0.55	0/1921
2	q	0.37	0/1423	0.55	0/1921
2	r	0.37	0/1423	0.55	0/1921
2	s	0.37	0/1423	0.55	0/1921
2	t	0.37	0/1423	0.55	0/1921
2	u	0.37	0/1423	0.55	0/1921
2	v	0.37	0/1423	0.55	0/1921
2	w	0.37	0/1423	0.55	0/1921
2	x	0.37	0/1423	0.55	0/1921
All	All	0.36	0/72024	0.53	24/97224 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	161	ARG	N-CA-C	-5.59	107.09	114.31
1	C	161	ARG	N-CA-C	-5.59	107.10	114.31
1	W	161	ARG	N-CA-C	-5.59	107.10	114.31
1	I	161	ARG	N-CA-C	-5.58	107.11	114.31
1	J	161	ARG	N-CA-C	-5.58	107.12	114.31
1	V	161	ARG	N-CA-C	-5.57	107.12	114.31
1	G	161	ARG	N-CA-C	-5.57	107.12	114.31
1	F	161	ARG	N-CA-C	-5.57	107.13	114.31
1	D	161	ARG	N-CA-C	-5.57	107.13	114.31
1	T	161	ARG	N-CA-C	-5.57	107.13	114.31
1	P	161	ARG	N-CA-C	-5.57	107.13	114.31
1	X	161	ARG	N-CA-C	-5.57	107.13	114.31
1	N	161	ARG	N-CA-C	-5.57	107.13	114.31
1	L	161	ARG	N-CA-C	-5.57	107.13	114.31
1	E	161	ARG	N-CA-C	-5.56	107.14	114.31
1	U	161	ARG	N-CA-C	-5.55	107.14	114.31
1	S	161	ARG	N-CA-C	-5.55	107.15	114.31
1	M	161	ARG	N-CA-C	-5.54	107.16	114.31
1	O	161	ARG	N-CA-C	-5.54	107.16	114.31
1	H	161	ARG	N-CA-C	-5.54	107.17	114.31
1	A	161	ARG	N-CA-C	-5.53	107.17	114.31
1	K	161	ARG	N-CA-C	-5.53	107.18	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ARG	N-CA-C	-5.53	107.18	114.31
1	R	161	ARG	N-CA-C	-5.53	107.18	114.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1554	0	1567	8	0
1	B	1554	0	1567	7	0
1	C	1554	0	1567	6	0
1	D	1554	0	1567	6	0
1	E	1554	0	1567	8	0
1	F	1554	0	1567	7	0
1	G	1554	0	1567	8	0
1	H	1554	0	1567	7	0
1	I	1554	0	1567	7	0
1	J	1554	0	1567	7	0
1	K	1554	0	1567	7	0
1	L	1554	0	1567	7	0
1	M	1554	0	1567	6	0
1	N	1554	0	1567	7	0
1	O	1554	0	1567	7	0
1	P	1554	0	1567	8	0
1	Q	1554	0	1567	8	0
1	R	1554	0	1567	12	0
1	S	1554	0	1567	12	0
1	T	1554	0	1567	7	0
1	U	1554	0	1567	8	0
1	V	1554	0	1567	6	0
1	W	1554	0	1567	7	0
1	X	1554	0	1567	9	0
2	a	1403	0	1428	15	0
2	b	1403	0	1428	21	0
2	c	1403	0	1428	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	1403	0	1428	14	0
2	e	1403	0	1428	19	0
2	f	1403	0	1428	20	0
2	g	1403	0	1428	15	0
2	h	1403	0	1428	13	0
2	i	1403	0	1428	14	0
2	j	1403	0	1428	15	0
2	k	1403	0	1428	16	0
2	l	1403	0	1428	15	0
2	m	1403	0	1428	13	0
2	n	1403	0	1428	14	0
2	o	1403	0	1428	17	0
2	p	1403	0	1428	18	0
2	q	1403	0	1428	15	0
2	r	1403	0	1428	16	0
2	s	1403	0	1428	14	0
2	t	1403	0	1428	13	0
2	u	1403	0	1428	14	0
2	v	1403	0	1428	16	0
2	w	1403	0	1428	21	0
2	x	1403	0	1428	16	0
All	All	70968	0	71880	469	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 3.

All (469) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:190:GLU:OE1	2:g:74:ARG:NH2	2.19	0.73
2:m:190:GLU:OE1	2:n:74:ARG:NH2	2.25	0.69
2:s:190:GLU:OE1	2:t:74:ARG:NH2	2.27	0.68
2:n:190:GLU:OE1	2:o:74:ARG:NH2	2.26	0.67
2:k:190:GLU:OE1	2:l:74:ARG:NH2	2.28	0.66
2:j:190:GLU:OE1	2:k:74:ARG:NH2	2.28	0.65
2:a:113:ARG:HG2	2:v:130:HIS:HE1	1.62	0.65
2:e:105:ARG:NH1	2:f:89:MET:O	2.30	0.64
1:S:183:TRP:CE3	2:p:44:ASN:HB2	2.33	0.63
2:c:113:ARG:HG2	2:d:130:HIS:HE1	1.63	0.63
2:o:190:GLU:OE1	2:p:74:ARG:NH2	2.32	0.62
1:S:318:ASN:HD21	2:o:159:SER:HB2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:190:GLU:OE1	2:i:74:ARG:NH2	2.33	0.61
2:e:113:ARG:HG2	2:f:130:HIS:HE1	1.64	0.61
1:R:183:TRP:CE3	2:o:44:ASN:HB2	2.36	0.61
1:G:298:ASN:HB2	1:F:286:THR:HG21	1.84	0.60
1:I:298:ASN:HB2	1:H:286:THR:HG21	1.83	0.60
2:b:74:ARG:NH2	2:w:190:GLU:OE1	2.34	0.59
2:l:190:GLU:OE1	2:m:74:ARG:NH2	2.36	0.58
1:R:312:GLU:HG3	2:o:163:VAL:HG13	1.85	0.58
2:v:105:ARG:NH1	2:w:89:MET:O	2.37	0.58
2:d:31:ARG:NH1	2:e:79:PRO:HG2	2.20	0.57
2:q:113:ARG:HG2	2:r:130:HIS:HE1	1.70	0.57
2:d:190:GLU:OE1	2:e:74:ARG:NH2	2.36	0.57
2:r:190:GLU:OE1	2:s:74:ARG:NH2	2.38	0.56
1:R:318:ASN:HD21	2:n:159:SER:HB2	1.70	0.55
2:e:103:LYS:HG3	2:f:135:LEU:HD23	1.88	0.55
1:T:318:ASN:HD21	2:p:159:SER:HB2	1.72	0.55
1:P:318:ASN:HD21	2:l:159:SER:HB2	1.72	0.55
2:i:190:GLU:OE1	2:j:74:ARG:NH2	2.40	0.54
2:q:190:GLU:OE1	2:r:74:ARG:NH2	2.40	0.54
1:T:278:ARG:NH1	1:T:332:TYR:OH	2.41	0.54
1:S:278:ARG:NH1	1:S:332:TYR:OH	2.41	0.54
1:N:278:ARG:NH1	1:N:332:TYR:OH	2.41	0.54
1:I:278:ARG:NH1	1:I:332:TYR:OH	2.41	0.54
1:X:278:ARG:NH1	1:X:332:TYR:OH	2.41	0.54
1:J:278:ARG:NH1	1:J:332:TYR:OH	2.41	0.54
1:C:278:ARG:NH1	1:C:332:TYR:OH	2.41	0.54
1:B:278:ARG:NH1	1:B:332:TYR:OH	2.41	0.54
1:Q:278:ARG:NH1	1:Q:332:TYR:OH	2.41	0.54
1:H:278:ARG:NH1	1:H:332:TYR:OH	2.41	0.54
1:R:278:ARG:NH1	1:R:332:TYR:OH	2.41	0.54
1:M:278:ARG:NH1	1:M:332:TYR:OH	2.41	0.54
1:A:278:ARG:NH1	1:A:332:TYR:OH	2.41	0.54
2:g:113:ARG:HG2	2:h:130:HIS:HE1	1.73	0.54
1:K:278:ARG:NH1	1:K:332:TYR:OH	2.41	0.53
1:G:278:ARG:NH1	1:G:332:TYR:OH	2.41	0.53
1:O:278:ARG:NH1	1:O:332:TYR:OH	2.41	0.53
1:D:278:ARG:NH1	1:D:332:TYR:OH	2.41	0.53
1:U:278:ARG:NH1	1:U:332:TYR:OH	2.41	0.53
1:L:278:ARG:NH1	1:L:332:TYR:OH	2.41	0.53
1:W:278:ARG:NH1	1:W:332:TYR:OH	2.41	0.53
1:E:278:ARG:NH1	1:E:332:TYR:OH	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ARG:NH1	1:F:332:TYR:OH	2.41	0.53
1:V:278:ARG:NH1	1:V:332:TYR:OH	2.41	0.53
1:P:278:ARG:NH1	1:P:332:TYR:OH	2.41	0.53
2:f:25:ILE:HD12	2:f:73:MET:HE1	1.92	0.52
2:a:25:ILE:HD12	2:a:73:MET:HE1	1.92	0.52
2:d:25:ILE:HD12	2:d:73:MET:HE1	1.92	0.52
2:v:25:ILE:HD12	2:v:73:MET:HE1	1.92	0.52
2:e:25:ILE:HD12	2:e:73:MET:HE1	1.92	0.52
2:g:25:ILE:HD12	2:g:73:MET:HE1	1.92	0.52
2:t:190:GLU:OE1	2:u:74:ARG:NH2	2.42	0.52
2:x:25:ILE:HD12	2:x:73:MET:HE1	1.92	0.52
2:c:25:ILE:HD12	2:c:73:MET:HE1	1.92	0.52
2:w:25:ILE:HD12	2:w:73:MET:HE1	1.92	0.52
2:b:25:ILE:HD12	2:b:73:MET:HE1	1.92	0.52
2:h:25:ILE:HD12	2:h:73:MET:HE1	1.92	0.52
2:u:25:ILE:HD12	2:u:73:MET:HE1	1.92	0.52
2:t:25:ILE:HD12	2:t:73:MET:HE1	1.92	0.52
2:i:25:ILE:HD12	2:i:73:MET:HE1	1.92	0.52
2:s:25:ILE:HD12	2:s:73:MET:HE1	1.92	0.51
2:j:25:ILE:HD12	2:j:73:MET:HE1	1.92	0.51
2:r:25:ILE:HD12	2:r:73:MET:HE1	1.92	0.51
2:u:113:ARG:HG2	2:x:130:HIS:HE1	1.76	0.51
2:k:25:ILE:HD12	2:k:73:MET:HE1	1.92	0.51
2:q:25:ILE:HD12	2:q:73:MET:HE1	1.92	0.51
2:s:171:LYS:NZ	2:s:177:VAL:O	2.44	0.51
2:b:171:LYS:NZ	2:b:177:VAL:O	2.44	0.51
2:l:25:ILE:HD12	2:l:73:MET:HE1	1.92	0.51
2:o:113:ARG:HG2	2:p:130:HIS:HE1	1.75	0.51
2:p:25:ILE:HD12	2:p:73:MET:HE1	1.92	0.51
2:e:171:LYS:NZ	2:e:177:VAL:O	2.44	0.51
2:m:73:MET:HG2	2:m:78:LEU:HD12	1.93	0.51
2:p:171:LYS:NZ	2:p:177:VAL:O	2.44	0.51
2:w:171:LYS:NZ	2:w:177:VAL:O	2.44	0.51
2:x:171:LYS:NZ	2:x:177:VAL:O	2.44	0.51
1:M:221:ASN:ND2	1:M:242:ARG:O	2.40	0.50
2:l:73:MET:HG2	2:l:78:LEU:HD12	1.94	0.50
2:o:25:ILE:HD12	2:o:73:MET:HE1	1.92	0.50
1:C:165:VAL:HG22	1:C:265:LYS:HE3	1.94	0.50
2:d:171:LYS:NZ	2:d:177:VAL:O	2.44	0.50
2:k:73:MET:HG2	2:k:78:LEU:HD12	1.94	0.50
2:m:25:ILE:HD12	2:m:73:MET:HE1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:25:ILE:HD12	2:n:73:MET:HE1	1.92	0.50
2:n:73:MET:HG2	2:n:78:LEU:HD12	1.94	0.50
2:t:171:LYS:NZ	2:t:177:VAL:O	2.44	0.50
2:o:171:LYS:NZ	2:o:177:VAL:O	2.44	0.50
2:c:73:MET:HG2	2:c:78:LEU:HD12	1.94	0.50
2:d:73:MET:HG2	2:d:78:LEU:HD12	1.94	0.50
2:e:73:MET:HG2	2:e:78:LEU:HD12	1.94	0.50
2:u:190:GLU:OE1	2:x:74:ARG:NH2	2.44	0.50
1:H:165:VAL:HG22	1:H:265:LYS:HE3	1.94	0.50
1:B:165:VAL:HG22	1:B:265:LYS:HE3	1.94	0.50
2:q:176:ASP:N	2:q:176:ASP:OD1	2.45	0.50
2:r:171:LYS:NZ	2:r:177:VAL:O	2.44	0.50
1:I:165:VAL:HG22	1:I:265:LYS:HE3	1.94	0.50
1:D:165:VAL:HG22	1:D:265:LYS:HE3	1.94	0.50
2:b:73:MET:HG2	2:b:78:LEU:HD12	1.94	0.50
2:e:87:SER:HB2	2:f:89:MET:HE2	1.94	0.50
2:h:171:LYS:NZ	2:h:177:VAL:O	2.44	0.50
2:j:73:MET:HG2	2:j:78:LEU:HD12	1.94	0.50
2:l:171:LYS:NZ	2:l:177:VAL:O	2.44	0.50
2:t:176:ASP:OD1	2:t:176:ASP:N	2.45	0.50
1:G:165:VAL:HG22	1:G:265:LYS:HE3	1.94	0.50
2:a:176:ASP:OD1	2:a:176:ASP:N	2.45	0.50
2:b:176:ASP:OD1	2:b:176:ASP:N	2.45	0.50
2:d:176:ASP:OD1	2:d:176:ASP:N	2.45	0.50
2:f:73:MET:HG2	2:f:78:LEU:HD12	1.94	0.50
2:g:30:GLN:OE1	2:g:49:LYS:NZ	2.41	0.50
2:i:171:LYS:NZ	2:i:177:VAL:O	2.44	0.50
2:o:73:MET:HG2	2:o:78:LEU:HD12	1.94	0.50
2:u:171:LYS:NZ	2:u:177:VAL:O	2.44	0.50
2:w:73:MET:HG2	2:w:78:LEU:HD12	1.93	0.50
2:b:113:ARG:HG2	2:c:130:HIS:HE1	1.75	0.50
2:m:171:LYS:NZ	2:m:177:VAL:O	2.44	0.50
1:R:312:GLU:HG3	2:o:163:VAL:CG1	2.41	0.50
2:b:105:ARG:NH1	2:c:89:MET:O	2.45	0.49
2:c:30:GLN:OE1	2:c:49:LYS:NZ	2.41	0.49
2:e:86:ILE:HB	2:e:108:SER:HB2	1.95	0.49
2:g:73:MET:HG2	2:g:78:LEU:HD12	1.93	0.49
2:i:73:MET:HG2	2:i:78:LEU:HD12	1.93	0.49
2:k:171:LYS:NZ	2:k:177:VAL:O	2.44	0.49
2:l:86:ILE:HB	2:l:108:SER:HB2	1.95	0.49
2:n:86:ILE:HB	2:n:108:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:165:VAL:HG22	1:J:265:LYS:HE3	1.93	0.49
1:E:165:VAL:HG22	1:E:265:LYS:HE3	1.94	0.49
2:a:73:MET:HG2	2:a:78:LEU:HD12	1.93	0.49
2:g:86:ILE:HB	2:g:108:SER:HB2	1.95	0.49
2:j:86:ILE:HB	2:j:108:SER:HB2	1.95	0.49
2:p:73:MET:HG2	2:p:78:LEU:HD12	1.94	0.49
2:v:171:LYS:NZ	2:v:177:VAL:O	2.44	0.49
2:w:176:ASP:OD1	2:w:176:ASP:N	2.45	0.49
1:A:165:VAL:HG22	1:A:265:LYS:HE3	1.94	0.49
2:d:86:ILE:HB	2:d:108:SER:HB2	1.94	0.49
2:i:86:ILE:HB	2:i:108:SER:HB2	1.95	0.49
2:o:86:ILE:HB	2:o:108:SER:HB2	1.94	0.49
2:v:73:MET:HG2	2:v:78:LEU:HD12	1.94	0.49
2:x:73:MET:HG2	2:x:78:LEU:HD12	1.93	0.49
2:h:86:ILE:HB	2:h:108:SER:HB2	1.95	0.49
2:s:176:ASP:OD1	2:s:176:ASP:N	2.45	0.49
2:u:73:MET:HG2	2:u:78:LEU:HD12	1.93	0.49
1:S:165:VAL:HG22	1:S:265:LYS:HE3	1.93	0.49
1:Q:165:VAL:HG22	1:Q:265:LYS:HE3	1.94	0.49
1:P:165:VAL:HG22	1:P:265:LYS:HE3	1.94	0.49
1:F:221:ASN:ND2	1:F:242:ARG:O	2.40	0.49
1:U:165:VAL:HG22	1:U:265:LYS:HE3	1.93	0.49
2:b:86:ILE:HB	2:b:108:SER:HB2	1.95	0.49
2:c:86:ILE:HB	2:c:108:SER:HB2	1.95	0.49
2:g:171:LYS:NZ	2:g:177:VAL:O	2.44	0.49
2:i:176:ASP:OD1	2:i:176:ASP:N	2.45	0.49
2:m:86:ILE:HB	2:m:108:SER:HB2	1.95	0.49
2:q:86:ILE:HB	2:q:108:SER:HB2	1.95	0.49
2:t:113:ARG:HG2	2:u:130:HIS:HE1	1.77	0.49
2:x:176:ASP:N	2:x:176:ASP:OD1	2.45	0.49
1:R:165:VAL:HG22	1:R:265:LYS:HE3	1.93	0.49
1:V:165:VAL:HG22	1:V:265:LYS:HE3	1.93	0.49
2:c:171:LYS:NZ	2:c:177:VAL:O	2.44	0.49
2:f:176:ASP:OD1	2:f:176:ASP:N	2.45	0.49
2:k:86:ILE:HB	2:k:108:SER:HB2	1.95	0.49
2:p:86:ILE:HB	2:p:108:SER:HB2	1.95	0.49
2:t:30:GLN:OE1	2:t:49:LYS:NZ	2.41	0.49
2:t:73:MET:HG2	2:t:78:LEU:HD12	1.93	0.49
1:N:165:VAL:HG22	1:N:265:LYS:HE3	1.93	0.49
1:A:221:ASN:ND2	1:A:242:ARG:O	2.40	0.49
1:X:165:VAL:HG22	1:X:265:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:129:ILE:HG12	2:b:149:VAL:HG12	1.95	0.49
2:d:129:ILE:HG12	2:d:149:VAL:HG12	1.95	0.49
2:f:86:ILE:HB	2:f:108:SER:HB2	1.95	0.49
2:n:171:LYS:NZ	2:n:177:VAL:O	2.44	0.49
2:n:176:ASP:OD1	2:n:176:ASP:N	2.45	0.49
1:O:221:ASN:ND2	1:O:242:ARG:O	2.40	0.49
1:F:165:VAL:HG22	1:F:265:LYS:HE3	1.93	0.49
2:a:130:HIS:HE1	2:x:113:ARG:HG2	1.78	0.49
2:h:73:MET:HG2	2:h:78:LEU:HD12	1.93	0.49
2:k:176:ASP:OD1	2:k:176:ASP:N	2.45	0.49
2:m:129:ILE:HG12	2:m:149:VAL:HG12	1.95	0.49
2:q:30:GLN:OE1	2:q:49:LYS:NZ	2.41	0.49
2:r:73:MET:HG2	2:r:78:LEU:HD12	1.93	0.49
2:s:73:MET:HG2	2:s:78:LEU:HD12	1.93	0.49
2:s:86:ILE:HB	2:s:108:SER:HB2	1.94	0.49
2:v:86:ILE:HB	2:v:108:SER:HB2	1.95	0.49
2:v:176:ASP:N	2:v:176:ASP:OD1	2.45	0.49
1:T:221:ASN:ND2	1:T:242:ARG:O	2.40	0.49
2:h:176:ASP:OD1	2:h:176:ASP:N	2.45	0.49
2:l:176:ASP:N	2:l:176:ASP:OD1	2.45	0.49
2:o:129:ILE:HG12	2:o:149:VAL:HG12	1.95	0.49
2:o:176:ASP:N	2:o:176:ASP:OD1	2.45	0.49
2:q:73:MET:HG2	2:q:78:LEU:HD12	1.94	0.49
2:v:129:ILE:HG12	2:v:149:VAL:HG12	1.95	0.49
2:w:86:ILE:HB	2:w:108:SER:HB2	1.94	0.49
2:x:86:ILE:HB	2:x:108:SER:HB2	1.94	0.49
2:x:129:ILE:HG12	2:x:149:VAL:HG12	1.95	0.49
2:c:176:ASP:OD1	2:c:176:ASP:N	2.45	0.49
2:f:129:ILE:HG12	2:f:149:VAL:HG12	1.95	0.49
2:i:145:MET:HB3	2:i:177:VAL:HG22	1.95	0.49
2:j:171:LYS:NZ	2:j:177:VAL:O	2.44	0.49
2:j:176:ASP:N	2:j:176:ASP:OD1	2.45	0.49
2:k:129:ILE:HG12	2:k:149:VAL:HG12	1.95	0.49
2:k:145:MET:HB3	2:k:177:VAL:HG22	1.95	0.49
2:p:176:ASP:OD1	2:p:176:ASP:N	2.45	0.49
2:r:86:ILE:HB	2:r:108:SER:HB2	1.95	0.49
2:u:86:ILE:HB	2:u:108:SER:HB2	1.95	0.49
1:S:182:VAL:HG23	2:o:192:TYR:CE2	2.48	0.48
1:O:165:VAL:HG22	1:O:265:LYS:HE3	1.94	0.48
1:M:165:VAL:HG22	1:M:265:LYS:HE3	1.93	0.48
2:a:86:ILE:HB	2:a:108:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:145:MET:HB3	2:m:177:VAL:HG22	1.95	0.48
2:p:145:MET:HB3	2:p:177:VAL:HG22	1.95	0.48
1:T:165:VAL:HG22	1:T:265:LYS:HE3	1.94	0.48
1:H:221:ASN:ND2	1:H:242:ARG:O	2.40	0.48
2:i:129:ILE:HG12	2:i:149:VAL:HG12	1.95	0.48
2:m:176:ASP:OD1	2:m:176:ASP:N	2.45	0.48
2:n:145:MET:HB3	2:n:177:VAL:HG22	1.95	0.48
2:q:129:ILE:HG12	2:q:149:VAL:HG12	1.95	0.48
2:t:86:ILE:HB	2:t:108:SER:HB2	1.95	0.48
1:K:165:VAL:HG22	1:K:265:LYS:HE3	1.93	0.48
2:g:145:MET:HB3	2:g:177:VAL:HG22	1.95	0.48
2:h:129:ILE:HG12	2:h:149:VAL:HG12	1.95	0.48
2:h:145:MET:HB3	2:h:177:VAL:HG22	1.95	0.48
2:l:145:MET:HB3	2:l:177:VAL:HG22	1.95	0.48
2:q:145:MET:HB3	2:q:177:VAL:HG22	1.95	0.48
2:q:171:LYS:NZ	2:q:177:VAL:O	2.44	0.48
2:r:145:MET:HB3	2:r:177:VAL:HG22	1.95	0.48
2:t:129:ILE:HG12	2:t:149:VAL:HG12	1.95	0.48
1:L:165:VAL:HG22	1:L:265:LYS:HE3	1.94	0.48
1:W:165:VAL:HG22	1:W:265:LYS:HE3	1.93	0.48
2:a:30:GLN:OE1	2:a:49:LYS:NZ	2.41	0.48
2:i:113:ARG:HG2	2:j:130:HIS:HE1	1.78	0.48
2:j:30:GLN:OE1	2:j:49:LYS:NZ	2.41	0.48
2:j:145:MET:HB3	2:j:177:VAL:HG22	1.95	0.48
2:o:145:MET:HB3	2:o:177:VAL:HG22	1.95	0.48
2:p:129:ILE:HG12	2:p:149:VAL:HG12	1.95	0.48
2:v:113:ARG:HG2	2:w:130:HIS:HE1	1.76	0.48
2:f:109:ALA:HB2	2:g:89:MET:HG3	1.96	0.48
2:f:145:MET:HB3	2:f:177:VAL:HG22	1.95	0.48
2:g:129:ILE:HG12	2:g:149:VAL:HG12	1.95	0.48
2:j:129:ILE:HG12	2:j:149:VAL:HG12	1.95	0.48
2:r:129:ILE:HG12	2:r:149:VAL:HG12	1.95	0.48
2:s:145:MET:HB3	2:s:177:VAL:HG22	1.95	0.48
2:b:83:ARG:HA	2:w:116:GLN:HE22	1.79	0.48
2:g:190:GLU:OE1	2:h:74:ARG:NH2	2.45	0.48
2:s:129:ILE:HG12	2:s:149:VAL:HG12	1.95	0.48
2:u:145:MET:HB3	2:u:177:VAL:HG22	1.95	0.48
2:d:145:MET:HB3	2:d:177:VAL:HG22	1.95	0.48
2:l:129:ILE:HG12	2:l:149:VAL:HG12	1.95	0.48
2:u:129:ILE:HG12	2:u:149:VAL:HG12	1.95	0.48
2:e:145:MET:HB3	2:e:177:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:171:LYS:NZ	2:f:177:VAL:O	2.44	0.48
2:t:145:MET:HB3	2:t:177:VAL:HG22	1.95	0.48
2:a:74:ARG:NH2	2:x:190:GLU:OE1	2.46	0.48
2:n:129:ILE:HG12	2:n:149:VAL:HG12	1.95	0.48
2:b:145:MET:HB3	2:b:177:VAL:HG22	1.95	0.47
2:c:129:ILE:HG12	2:c:149:VAL:HG12	1.95	0.47
2:c:145:MET:HB3	2:c:177:VAL:HG22	1.95	0.47
2:u:176:ASP:OD1	2:u:176:ASP:N	2.45	0.47
2:a:145:MET:HB3	2:a:177:VAL:HG22	1.95	0.47
2:e:129:ILE:HG12	2:e:149:VAL:HG12	1.95	0.47
2:a:129:ILE:HG12	2:a:149:VAL:HG12	1.95	0.47
1:Q:221:ASN:ND2	1:Q:242:ARG:O	2.40	0.47
2:a:171:LYS:NZ	2:a:177:VAL:O	2.44	0.47
2:v:145:MET:HB3	2:v:177:VAL:HG22	1.95	0.47
2:w:129:ILE:HG12	2:w:149:VAL:HG12	1.95	0.47
2:w:145:MET:HB3	2:w:177:VAL:HG22	1.95	0.47
2:x:145:MET:HB3	2:x:177:VAL:HG22	1.96	0.47
1:J:221:ASN:ND2	1:J:242:ARG:O	2.40	0.47
1:U:221:ASN:ND2	1:U:242:ARG:O	2.40	0.47
2:f:30:GLN:OE1	2:f:49:LYS:NZ	2.41	0.47
2:v:190:GLU:OE1	2:w:74:ARG:NH2	2.46	0.47
1:S:221:ASN:ND2	1:S:242:ARG:O	2.40	0.47
1:C:221:ASN:ND2	1:C:242:ARG:O	2.40	0.47
2:r:176:ASP:OD1	2:r:176:ASP:N	2.45	0.47
2:m:109:ALA:HB2	2:n:89:MET:HG3	1.97	0.47
2:m:30:GLN:OE1	2:m:49:LYS:NZ	2.41	0.47
1:N:221:ASN:ND2	1:N:242:ARG:O	2.40	0.47
2:d:37:ILE:HG21	2:e:66:PHE:HE2	1.80	0.46
2:e:176:ASP:N	2:e:176:ASP:OD1	2.45	0.46
1:A:158:ASP:OD1	1:A:158:ASP:N	2.49	0.46
1:P:221:ASN:ND2	1:P:242:ARG:O	2.40	0.46
1:B:158:ASP:N	1:B:158:ASP:OD1	2.49	0.46
2:b:30:GLN:OE1	2:b:49:LYS:NZ	2.41	0.46
1:L:221:ASN:ND2	1:L:242:ARG:O	2.40	0.46
2:b:130:HIS:CD2	2:w:169:PHE:HZ	2.34	0.46
2:p:30:GLN:OE1	2:p:49:LYS:NZ	2.41	0.46
2:b:66:PHE:HE2	2:w:37:ILE:HG21	1.80	0.46
2:e:175:SER:O	2:f:146:HIS:NE2	2.49	0.46
2:b:83:ARG:HA	2:w:116:GLN:NE2	2.31	0.46
2:e:169:PHE:HB2	2:f:185:ILE:HD12	1.98	0.46
2:g:176:ASP:N	2:g:176:ASP:OD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:113:ARG:HG2	2:i:130:HIS:HE1	1.81	0.46
2:s:30:GLN:OE1	2:s:49:LYS:NZ	2.41	0.46
1:W:158:ASP:OD1	1:W:158:ASP:N	2.49	0.45
1:V:158:ASP:N	1:V:158:ASP:OD1	2.49	0.45
2:i:30:GLN:OE1	2:i:49:LYS:NZ	2.41	0.45
1:C:158:ASP:OD1	1:C:158:ASP:N	2.49	0.45
2:w:30:GLN:OE1	2:w:49:LYS:NZ	2.41	0.45
1:S:183:TRP:CD2	2:p:44:ASN:HB2	2.51	0.45
1:O:318:ASN:HD21	2:k:159:SER:HB2	1.81	0.45
1:K:158:ASP:OD1	1:K:158:ASP:N	2.49	0.45
1:L:158:ASP:N	1:L:158:ASP:OD1	2.49	0.45
1:E:221:ASN:ND2	1:E:242:ARG:O	2.40	0.45
1:X:221:ASN:ND2	1:X:242:ARG:O	2.40	0.45
1:J:158:ASP:OD1	1:J:158:ASP:N	2.49	0.45
2:x:30:GLN:OE1	2:x:49:LYS:NZ	2.41	0.45
1:R:221:ASN:ND2	1:R:242:ARG:O	2.40	0.45
1:N:224:VAL:HG12	1:N:237:PHE:HB2	1.99	0.45
1:M:224:VAL:HG12	1:M:237:PHE:HB2	1.99	0.45
1:T:158:ASP:OD1	1:T:158:ASP:N	2.49	0.45
1:P:224:VAL:HG12	1:P:237:PHE:HB2	1.99	0.45
1:M:158:ASP:OD1	1:M:158:ASP:N	2.49	0.45
1:K:318:ASN:HD21	2:g:159:SER:HB2	1.82	0.45
1:E:158:ASP:N	1:E:158:ASP:OD1	2.49	0.45
1:B:224:VAL:HG12	1:B:237:PHE:HB2	1.99	0.45
1:V:224:VAL:HG12	1:V:237:PHE:HB2	1.99	0.45
1:X:224:VAL:HG12	1:X:237:PHE:HB2	1.99	0.45
2:e:169:PHE:HB2	2:f:185:ILE:CD1	2.47	0.45
2:v:30:GLN:OE1	2:v:49:LYS:NZ	2.41	0.45
1:S:224:VAL:HG12	1:S:237:PHE:HB2	1.99	0.44
1:R:224:VAL:HG12	1:R:237:PHE:HB2	1.99	0.44
1:P:158:ASP:OD1	1:P:158:ASP:N	2.49	0.44
1:L:224:VAL:HG12	1:L:237:PHE:HB2	1.99	0.44
1:K:224:VAL:HG12	1:K:237:PHE:HB2	1.99	0.44
1:W:221:ASN:ND2	1:W:242:ARG:O	2.40	0.44
1:W:224:VAL:HG12	1:W:237:PHE:HB2	1.99	0.44
1:Q:158:ASP:N	1:Q:158:ASP:OD1	2.49	0.44
1:Q:318:ASN:HD21	2:m:159:SER:HB2	1.82	0.44
1:E:182:VAL:HG11	2:b:43:HIS:ND1	2.33	0.44
1:D:224:VAL:HG12	1:D:237:PHE:HB2	1.99	0.44
1:A:224:VAL:HG12	1:A:237:PHE:HB2	1.99	0.44
1:U:224:VAL:HG12	1:U:237:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:158:ASP:N	1:X:158:ASP:OD1	2.49	0.44
1:S:158:ASP:N	1:S:158:ASP:OD1	2.49	0.44
1:Q:224:VAL:HG12	1:Q:237:PHE:HB2	1.99	0.44
1:O:224:VAL:HG12	1:O:237:PHE:HB2	1.99	0.44
1:L:205:GLU:OE1	1:L:263:TYR:OH	2.30	0.44
1:O:158:ASP:OD1	1:O:158:ASP:N	2.49	0.44
1:I:158:ASP:OD1	1:I:158:ASP:N	2.49	0.44
1:I:224:VAL:HG12	1:I:237:PHE:HB2	1.99	0.44
1:C:224:VAL:HG12	1:C:237:PHE:HB2	1.99	0.44
1:T:224:VAL:HG12	1:T:237:PHE:HB2	1.99	0.44
2:a:105:ARG:NH1	2:v:89:MET:O	2.50	0.44
2:j:105:ARG:NH1	2:k:89:MET:O	2.51	0.44
1:R:158:ASP:OD1	1:R:158:ASP:N	2.49	0.44
1:J:205:GLU:OE1	1:J:263:TYR:OH	2.30	0.44
1:J:224:VAL:HG12	1:J:237:PHE:HB2	1.99	0.44
1:G:224:VAL:HG12	1:G:237:PHE:HB2	1.99	0.44
1:F:224:VAL:HG12	1:F:237:PHE:HB2	1.99	0.44
1:E:224:VAL:HG12	1:E:237:PHE:HB2	2.00	0.44
2:e:30:GLN:OE1	2:e:49:LYS:NZ	2.41	0.44
1:T:220:ILE:HD13	1:T:253:LEU:HD22	2.00	0.44
1:I:220:ILE:HD13	1:I:253:LEU:HD22	2.00	0.44
1:H:224:VAL:HG12	1:H:237:PHE:HB2	2.00	0.44
2:h:30:GLN:OE1	2:h:49:LYS:NZ	2.41	0.44
2:o:30:GLN:OE1	2:o:49:LYS:NZ	2.41	0.44
1:N:158:ASP:N	1:N:158:ASP:OD1	2.49	0.44
1:J:220:ILE:HD13	1:J:253:LEU:HD22	2.00	0.44
1:F:220:ILE:HD13	1:F:253:LEU:HD22	2.00	0.44
1:W:220:ILE:HD13	1:W:253:LEU:HD22	2.00	0.44
1:G:221:ASN:ND2	1:G:242:ARG:O	2.40	0.43
1:E:220:ILE:HD13	1:E:253:LEU:HD22	2.00	0.43
1:A:220:ILE:HD13	1:A:253:LEU:HD22	2.00	0.43
1:P:220:ILE:HD13	1:P:253:LEU:HD22	2.00	0.43
1:U:179:ASN:OD1	2:s:43:HIS:ND1	2.51	0.43
1:X:220:ILE:HD13	1:X:253:LEU:HD22	2.00	0.43
1:S:220:ILE:HD13	1:S:253:LEU:HD22	2.00	0.43
1:M:220:ILE:HD13	1:M:253:LEU:HD22	2.00	0.43
1:H:158:ASP:OD1	1:H:158:ASP:N	2.49	0.43
1:Q:220:ILE:HD13	1:Q:253:LEU:HD22	2.00	0.43
1:D:158:ASP:OD1	1:D:158:ASP:N	2.49	0.43
1:D:220:ILE:HD13	1:D:253:LEU:HD22	2.00	0.43
2:l:30:GLN:OE1	2:l:49:LYS:NZ	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:220:ILE:HD13	1:N:253:LEU:HD22	2.00	0.43
1:K:220:ILE:HD13	1:K:253:LEU:HD22	2.00	0.43
1:G:158:ASP:N	1:G:158:ASP:OD1	2.49	0.43
1:V:220:ILE:HD13	1:V:253:LEU:HD22	2.00	0.43
2:k:113:ARG:HG2	2:l:130:HIS:HE1	1.83	0.43
2:p:109:ALA:HB2	2:q:89:MET:HG3	2.01	0.43
1:F:158:ASP:OD1	1:F:158:ASP:N	2.49	0.43
1:E:187:ALA:HB2	2:b:44:ASN:ND2	2.34	0.43
1:L:220:ILE:HD13	1:L:253:LEU:HD22	2.00	0.43
1:H:220:ILE:HD13	1:H:253:LEU:HD22	2.00	0.43
2:s:109:ALA:HB2	2:t:89:MET:HG3	2.01	0.43
1:N:205:GLU:OE1	1:N:263:TYR:OH	2.30	0.43
1:K:221:ASN:ND2	1:K:242:ARG:O	2.40	0.43
1:G:205:GLU:OE1	1:G:263:TYR:OH	2.30	0.43
1:G:220:ILE:HD13	1:G:253:LEU:HD22	2.00	0.43
1:B:220:ILE:HD13	1:B:253:LEU:HD22	2.00	0.43
2:c:103:LYS:HG3	2:d:135:LEU:HD23	2.00	0.43
2:k:30:GLN:OE1	2:k:49:LYS:NZ	2.41	0.42
2:k:105:ARG:NH1	2:l:89:MET:O	2.52	0.42
2:p:190:GLU:OE1	2:q:74:ARG:NH2	2.49	0.42
1:S:179:ASN:OD1	2:p:43:HIS:ND1	2.53	0.42
1:O:220:ILE:HD13	1:O:253:LEU:HD22	2.00	0.42
1:R:220:ILE:HD13	1:R:253:LEU:HD22	2.00	0.42
2:f:105:ARG:NH1	2:g:89:MET:O	2.53	0.42
1:U:220:ILE:HD13	1:U:253:LEU:HD22	2.00	0.42
1:I:221:ASN:ND2	1:I:242:ARG:O	2.40	0.42
1:C:220:ILE:HD13	1:C:253:LEU:HD22	2.00	0.42
1:A:318:ASN:HD21	2:u:159:SER:HB2	1.84	0.42
1:V:221:ASN:ND2	1:V:242:ARG:O	2.40	0.42
2:b:89:MET:HG3	2:w:109:ALA:HB2	2.02	0.42
2:j:109:ALA:HB2	2:k:89:MET:HG3	2.02	0.42
1:X:223:TYR:OH	1:X:274:ASP:OD1	2.31	0.42
2:j:111:GLU:OE1	2:j:133:TYR:OH	2.36	0.42
1:X:325:LYS:HG3	2:q:160:GLU:HG3	2.01	0.42
2:n:30:GLN:OE1	2:n:49:LYS:NZ	2.41	0.42
1:Q:205:GLU:OE1	1:Q:263:TYR:OH	2.30	0.41
1:B:221:ASN:ND2	1:B:242:ARG:O	2.40	0.41
1:B:318:ASN:HD21	2:x:159:SER:HB2	1.85	0.41
2:v:111:GLU:OE1	2:v:133:TYR:OH	2.36	0.41
2:f:78:LEU:HD23	2:f:78:LEU:HA	1.91	0.41
1:S:223:TYR:OH	1:S:274:ASP:OD1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:318:ASN:HD21	2:r:159:SER:HB2	1.85	0.41
2:n:152:ILE:HA	2:n:187:THR:O	2.21	0.41
2:r:30:GLN:OE1	2:r:49:LYS:NZ	2.41	0.41
2:u:30:GLN:OE1	2:u:49:LYS:NZ	2.41	0.41
2:m:152:ILE:HA	2:m:187:THR:O	2.21	0.41
2:t:152:ILE:HA	2:t:187:THR:O	2.21	0.41
2:w:111:GLU:OE1	2:w:133:TYR:OH	2.36	0.41
2:x:111:GLU:OE1	2:x:133:TYR:OH	2.36	0.41
2:u:152:ILE:HA	2:u:187:THR:O	2.21	0.41
1:W:223:TYR:OH	1:W:274:ASP:OD1	2.32	0.41
2:o:152:ILE:HA	2:o:187:THR:O	2.21	0.41
2:p:152:ILE:HA	2:p:187:THR:O	2.21	0.41
2:s:152:ILE:HA	2:s:187:THR:O	2.21	0.41
1:R:182:VAL:HG23	2:n:192:TYR:CE2	2.55	0.41
1:P:205:GLU:OE1	1:P:263:TYR:OH	2.30	0.41
1:U:158:ASP:OD1	1:U:158:ASP:N	2.49	0.41
2:a:169:PHE:HB2	2:v:185:ILE:CD1	2.50	0.41
2:c:111:GLU:OE1	2:c:133:TYR:OH	2.36	0.41
2:d:30:GLN:OE1	2:d:49:LYS:NZ	2.41	0.41
2:l:152:ILE:HA	2:l:187:THR:O	2.21	0.41
2:x:152:ILE:HA	2:x:187:THR:O	2.21	0.41
2:h:152:ILE:HA	2:h:187:THR:O	2.21	0.41
2:i:105:ARG:NH1	2:j:89:MET:O	2.53	0.41
2:v:31:ARG:NH1	2:w:79:PRO:HG2	2.36	0.41
2:a:111:GLU:OE1	2:a:133:TYR:OH	2.36	0.40
2:r:152:ILE:HA	2:r:187:THR:O	2.21	0.40
1:R:223:TYR:OH	1:R:274:ASP:OD1	2.32	0.40
2:b:111:GLU:OE1	2:b:133:TYR:OH	2.36	0.40
2:e:113:ARG:NH2	2:f:115:GLU:OE1	2.54	0.40
2:g:152:ILE:HA	2:g:187:THR:O	2.21	0.40
2:i:152:ILE:HA	2:i:187:THR:O	2.21	0.40
2:p:105:ARG:NH1	2:q:89:MET:O	2.55	0.40
1:A:223:TYR:OH	1:A:274:ASP:OD1	2.31	0.40
2:a:89:MET:O	2:x:105:ARG:NH1	2.54	0.40
2:b:152:ILE:HA	2:b:187:THR:O	2.21	0.40
2:d:152:ILE:HA	2:d:187:THR:O	2.21	0.40
2:r:113:ARG:HG2	2:s:130:HIS:HE1	1.86	0.40
2:w:152:ILE:HA	2:w:187:THR:O	2.21	0.40
1:X:183:TRP:CE3	2:r:44:ASN:HB2	2.56	0.40
2:c:152:ILE:HA	2:c:187:THR:O	2.21	0.40
2:w:78:LEU:HD23	2:w:78:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ASN:ND2	1:D:242:ARG:O	2.40	0.40
2:b:78:LEU:O	2:b:80:ASN:N	2.55	0.40
2:k:152:ILE:HA	2:k:187:THR:O	2.21	0.40
2:l:111:GLU:OE1	2:l:133:TYR:OH	2.36	0.40
2:q:152:ILE:HA	2:q:187:THR:O	2.21	0.40
2:r:78:LEU:HA	2:r:78:LEU:HD23	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	B	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	C	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	D	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	E	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	F	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	G	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	H	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	I	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	J	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	K	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	L	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	M	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	N	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	O	187/371 (50%)	177 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	Q	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	R	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	S	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	T	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	U	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	V	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	W	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
1	X	187/371 (50%)	177 (95%)	10 (5%)	0	100	100
2	a	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	b	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	c	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	d	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	e	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	f	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	g	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	h	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	i	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	j	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	k	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	l	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	m	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	n	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	o	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	p	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	q	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	r	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	s	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	t	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	u	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	v	175/241 (73%)	155 (89%)	20 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	w	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
2	x	175/241 (73%)	155 (89%)	20 (11%)	0	100	100
All	All	8688/14688 (59%)	7968 (92%)	720 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	174/342 (51%)	174 (100%)	0	100	100
1	B	174/342 (51%)	174 (100%)	0	100	100
1	C	174/342 (51%)	174 (100%)	0	100	100
1	D	174/342 (51%)	174 (100%)	0	100	100
1	E	174/342 (51%)	174 (100%)	0	100	100
1	F	174/342 (51%)	174 (100%)	0	100	100
1	G	174/342 (51%)	174 (100%)	0	100	100
1	H	174/342 (51%)	174 (100%)	0	100	100
1	I	174/342 (51%)	174 (100%)	0	100	100
1	J	174/342 (51%)	174 (100%)	0	100	100
1	K	174/342 (51%)	174 (100%)	0	100	100
1	L	174/342 (51%)	174 (100%)	0	100	100
1	M	174/342 (51%)	174 (100%)	0	100	100
1	N	174/342 (51%)	174 (100%)	0	100	100
1	O	174/342 (51%)	174 (100%)	0	100	100
1	P	174/342 (51%)	174 (100%)	0	100	100
1	Q	174/342 (51%)	174 (100%)	0	100	100
1	R	174/342 (51%)	174 (100%)	0	100	100
1	S	174/342 (51%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	174/342 (51%)	174 (100%)	0	100	100
1	U	174/342 (51%)	174 (100%)	0	100	100
1	V	174/342 (51%)	174 (100%)	0	100	100
1	W	174/342 (51%)	174 (100%)	0	100	100
1	X	174/342 (51%)	174 (100%)	0	100	100
2	a	162/220 (74%)	162 (100%)	0	100	100
2	b	162/220 (74%)	162 (100%)	0	100	100
2	c	162/220 (74%)	162 (100%)	0	100	100
2	d	162/220 (74%)	162 (100%)	0	100	100
2	e	162/220 (74%)	162 (100%)	0	100	100
2	f	162/220 (74%)	162 (100%)	0	100	100
2	g	162/220 (74%)	162 (100%)	0	100	100
2	h	162/220 (74%)	162 (100%)	0	100	100
2	i	162/220 (74%)	162 (100%)	0	100	100
2	j	162/220 (74%)	162 (100%)	0	100	100
2	k	162/220 (74%)	162 (100%)	0	100	100
2	l	162/220 (74%)	162 (100%)	0	100	100
2	m	162/220 (74%)	162 (100%)	0	100	100
2	n	162/220 (74%)	162 (100%)	0	100	100
2	o	162/220 (74%)	162 (100%)	0	100	100
2	p	162/220 (74%)	162 (100%)	0	100	100
2	q	162/220 (74%)	162 (100%)	0	100	100
2	r	162/220 (74%)	162 (100%)	0	100	100
2	s	162/220 (74%)	162 (100%)	0	100	100
2	t	162/220 (74%)	162 (100%)	0	100	100
2	u	162/220 (74%)	162 (100%)	0	100	100
2	v	162/220 (74%)	162 (100%)	0	100	100
2	w	162/220 (74%)	162 (100%)	0	100	100
2	x	162/220 (74%)	162 (100%)	0	100	100
All	All	8064/13488 (60%)	8064 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	318	ASN
1	S	324	HIS
1	T	318	ASN
1	T	324	HIS
1	R	318	ASN
1	R	324	HIS
1	Q	318	ASN
1	Q	324	HIS
1	P	318	ASN
1	P	324	HIS
1	O	318	ASN
1	N	318	ASN
1	N	324	HIS
1	M	318	ASN
1	M	324	HIS
1	K	318	ASN
1	K	324	HIS
1	J	324	HIS
1	I	324	HIS
1	H	324	HIS
1	G	324	HIS
1	F	324	HIS
1	E	324	HIS
1	D	324	HIS
1	C	324	HIS
1	B	318	ASN
1	A	318	ASN
1	A	324	HIS
1	W	318	ASN
1	W	324	HIS
1	V	318	ASN
1	V	324	HIS
1	U	318	ASN
1	U	324	HIS
1	X	324	HIS
2	a	165	ASN
2	b	165	ASN
2	c	130	HIS
2	c	165	ASN
2	d	165	ASN
2	e	130	HIS

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Mol	Chain	Res	Type
2	e	165	ASN
2	f	130	HIS
2	f	165	ASN
2	g	130	HIS
2	g	165	ASN
2	h	165	ASN
2	i	130	HIS
2	i	165	ASN
2	j	130	HIS
2	j	165	ASN
2	k	130	HIS
2	k	165	ASN
2	l	130	HIS
2	l	165	ASN
2	m	165	ASN
2	n	130	HIS
2	n	165	ASN
2	o	130	HIS
2	o	165	ASN
2	p	165	ASN
2	q	130	HIS
2	r	130	HIS
2	r	165	ASN
2	s	165	ASN
2	t	130	HIS
2	t	165	ASN
2	u	130	HIS
2	u	165	ASN
2	v	130	HIS
2	v	165	ASN
2	w	130	HIS
2	w	165	ASN
2	x	130	HIS
2	x	165	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

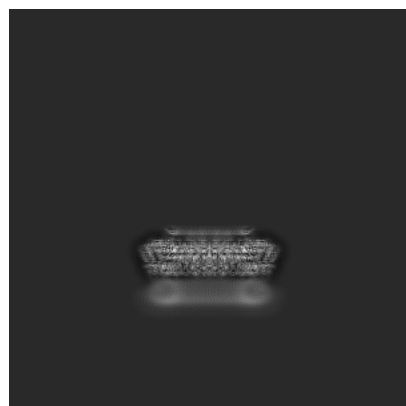
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10045. These allow visual inspection of the internal detail of the map and identification of artifacts.

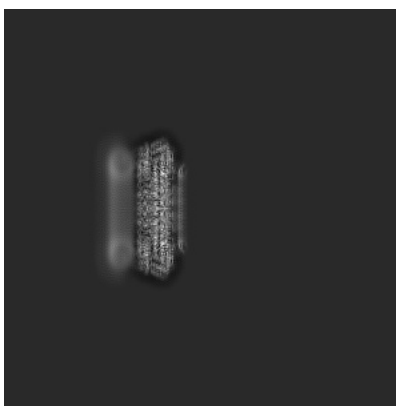
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

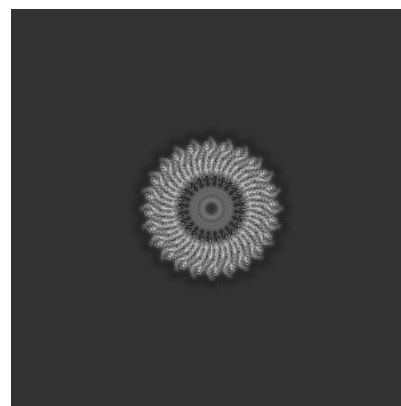
6.1.1 Primary map



X

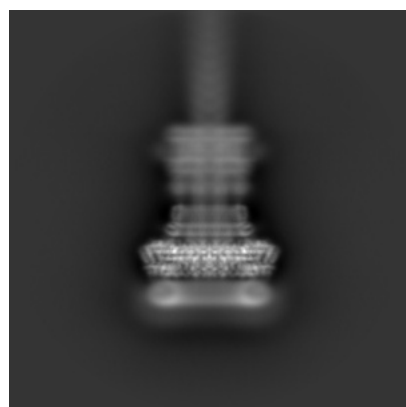


Y



Z

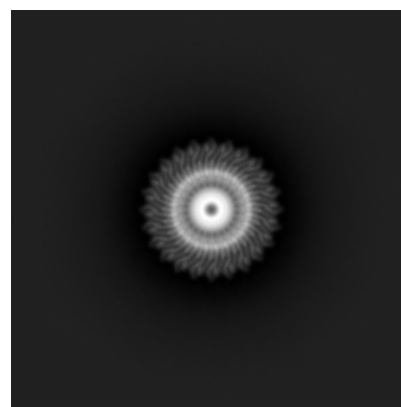
6.1.2 Raw map



X



Y

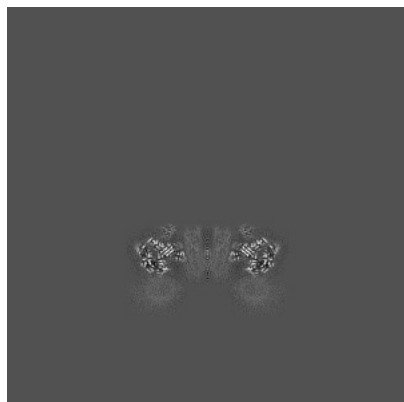


Z

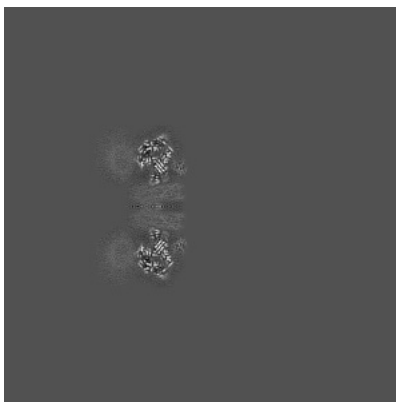
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

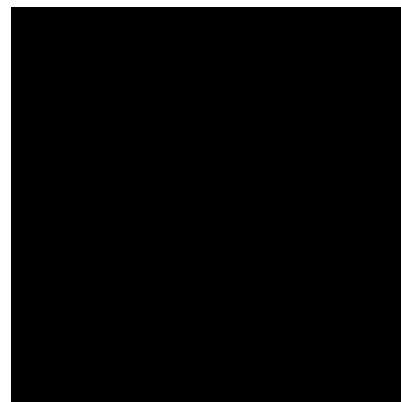
6.2.1 Primary map



X Index: 240

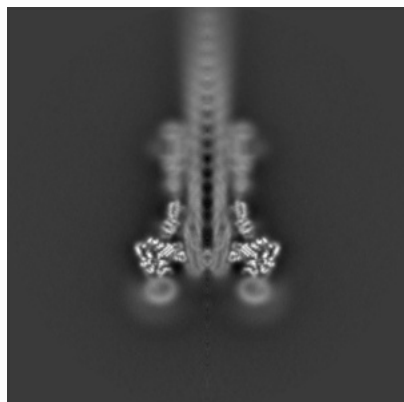


Y Index: 240

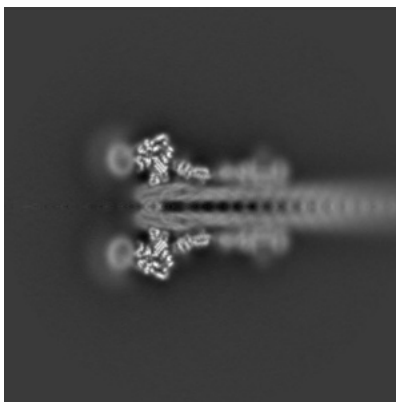


Z Index: 240

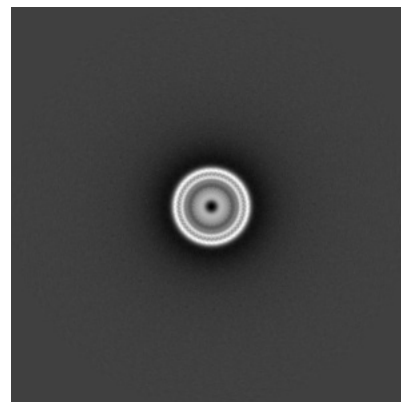
6.2.2 Raw map



X Index: 240



Y Index: 240

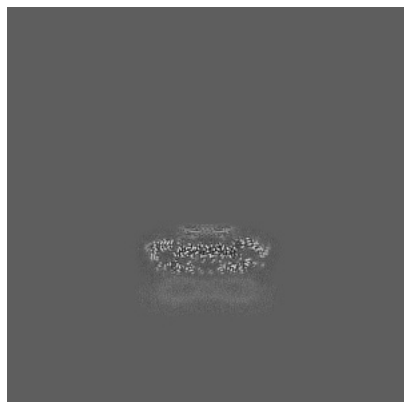


Z Index: 240

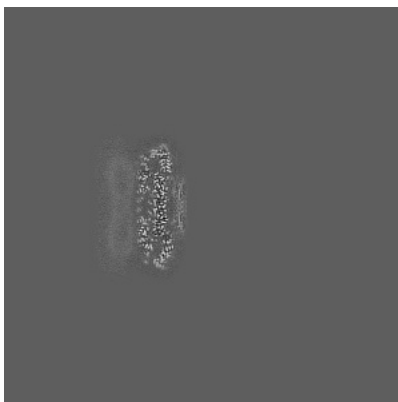
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

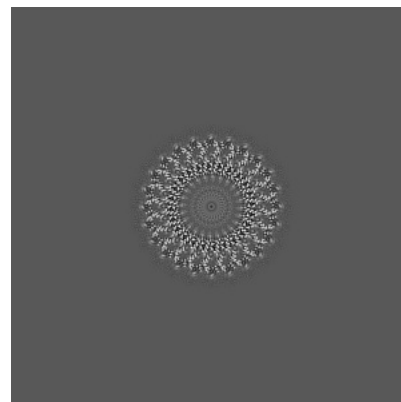
6.3.1 Primary map



X Index: 283

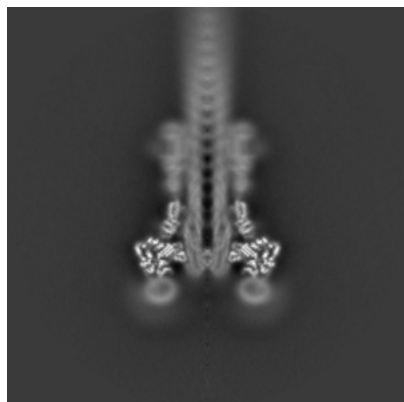


Y Index: 283

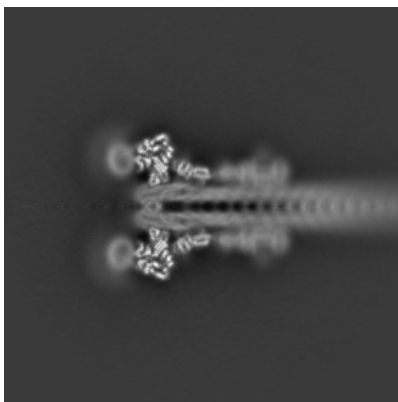


Z Index: 189

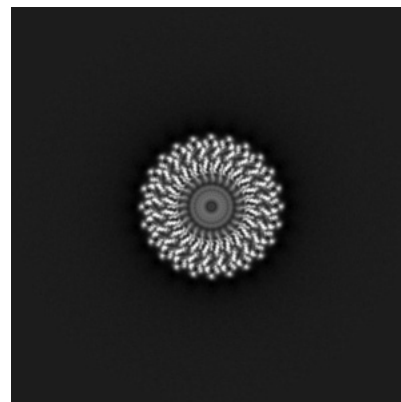
6.3.2 Raw map



X Index: 240



Y Index: 240

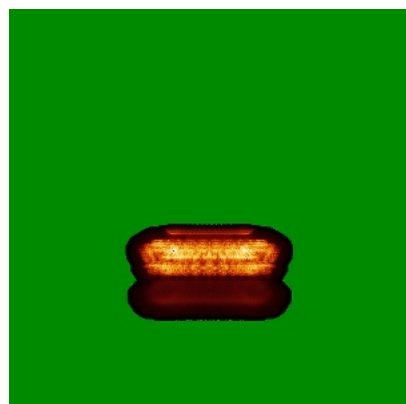


Z Index: 189

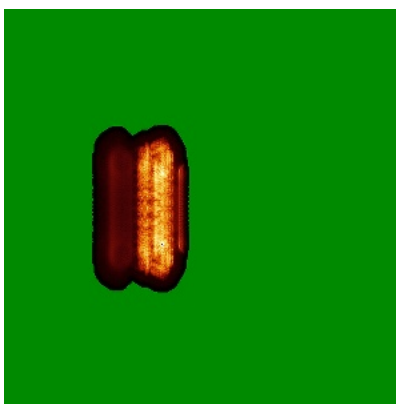
The images above show the largest variance slices of the map in three orthogonal directions.

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

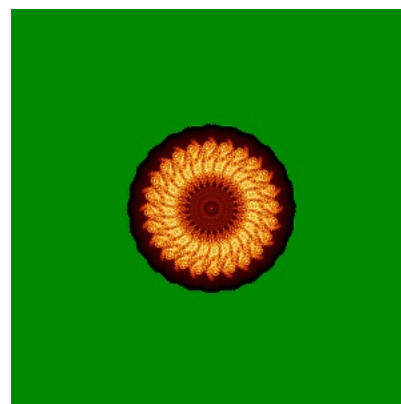
6.4.1 Primary map



X

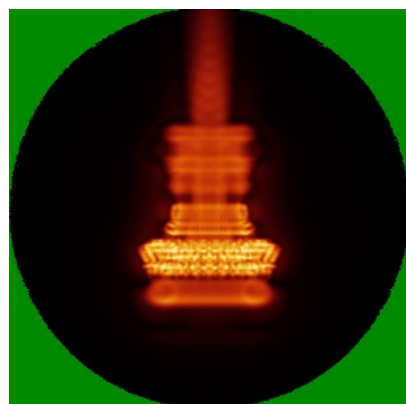


Y

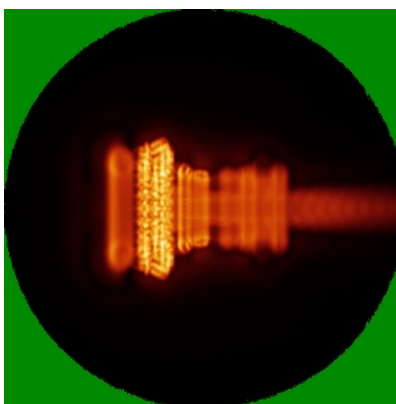


Z

6.4.2 Raw map



X



Y

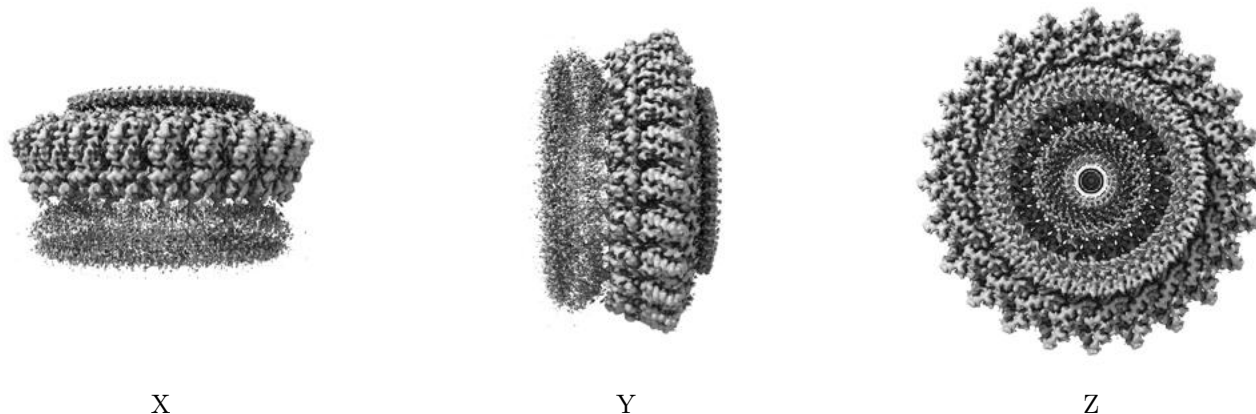


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

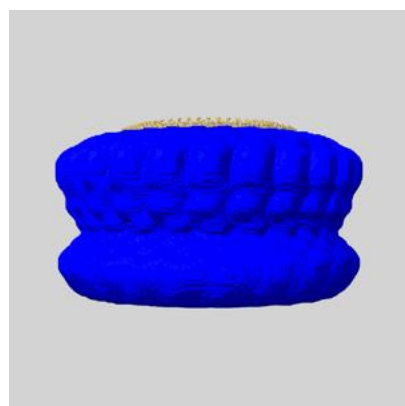
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

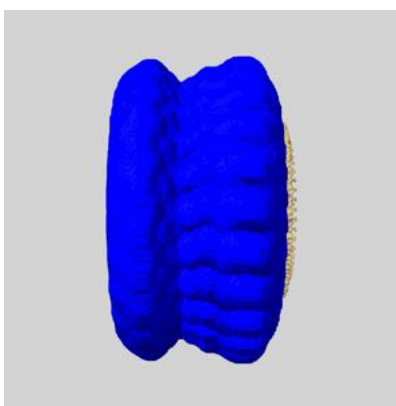
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

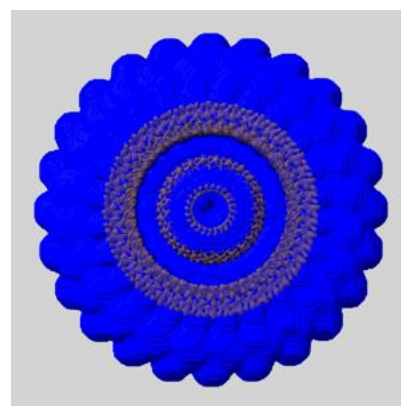
6.6.1 emd_10045_msk_1.map [i](#)



X



Y

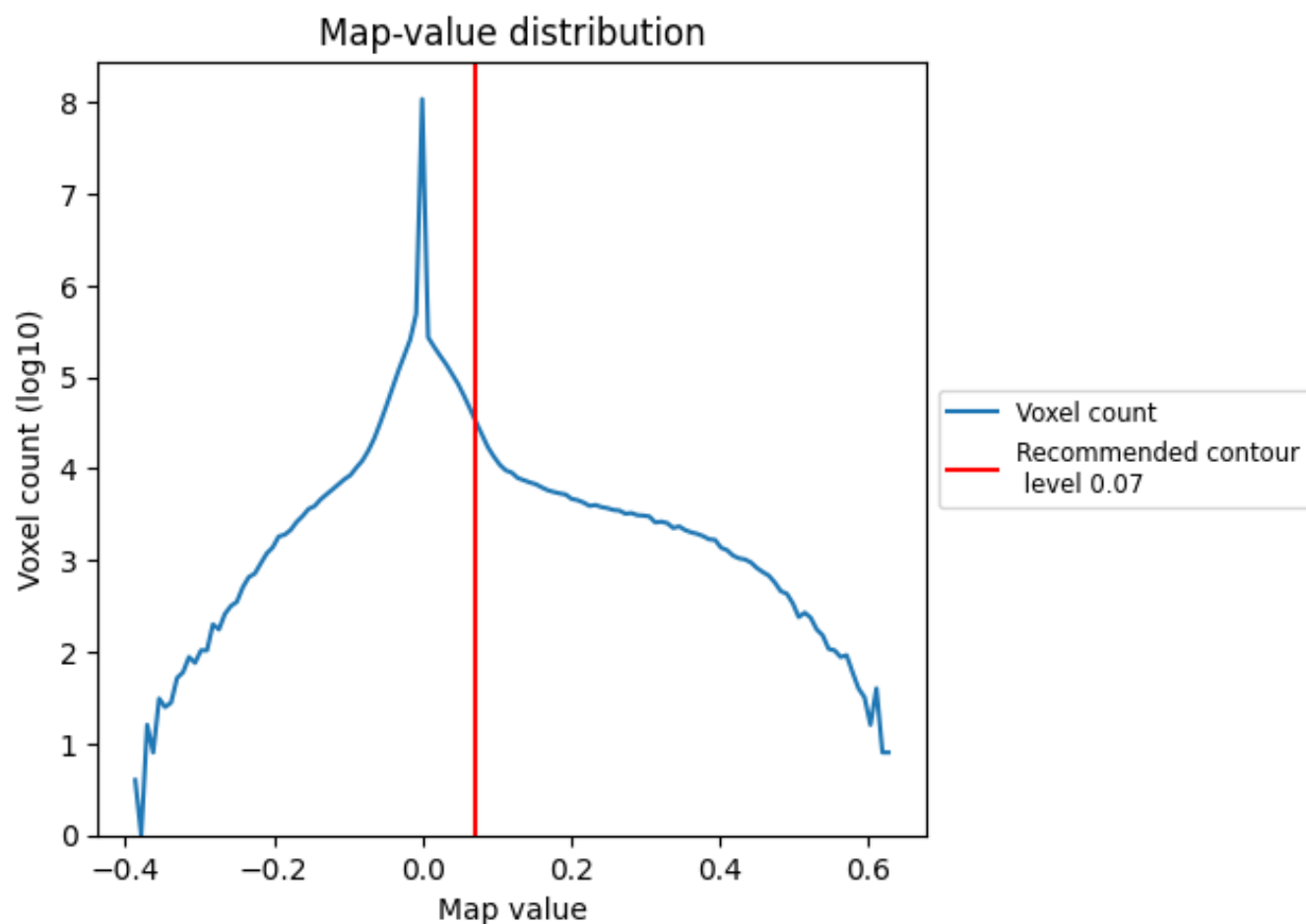


Z

7 Map analysis [i](#)

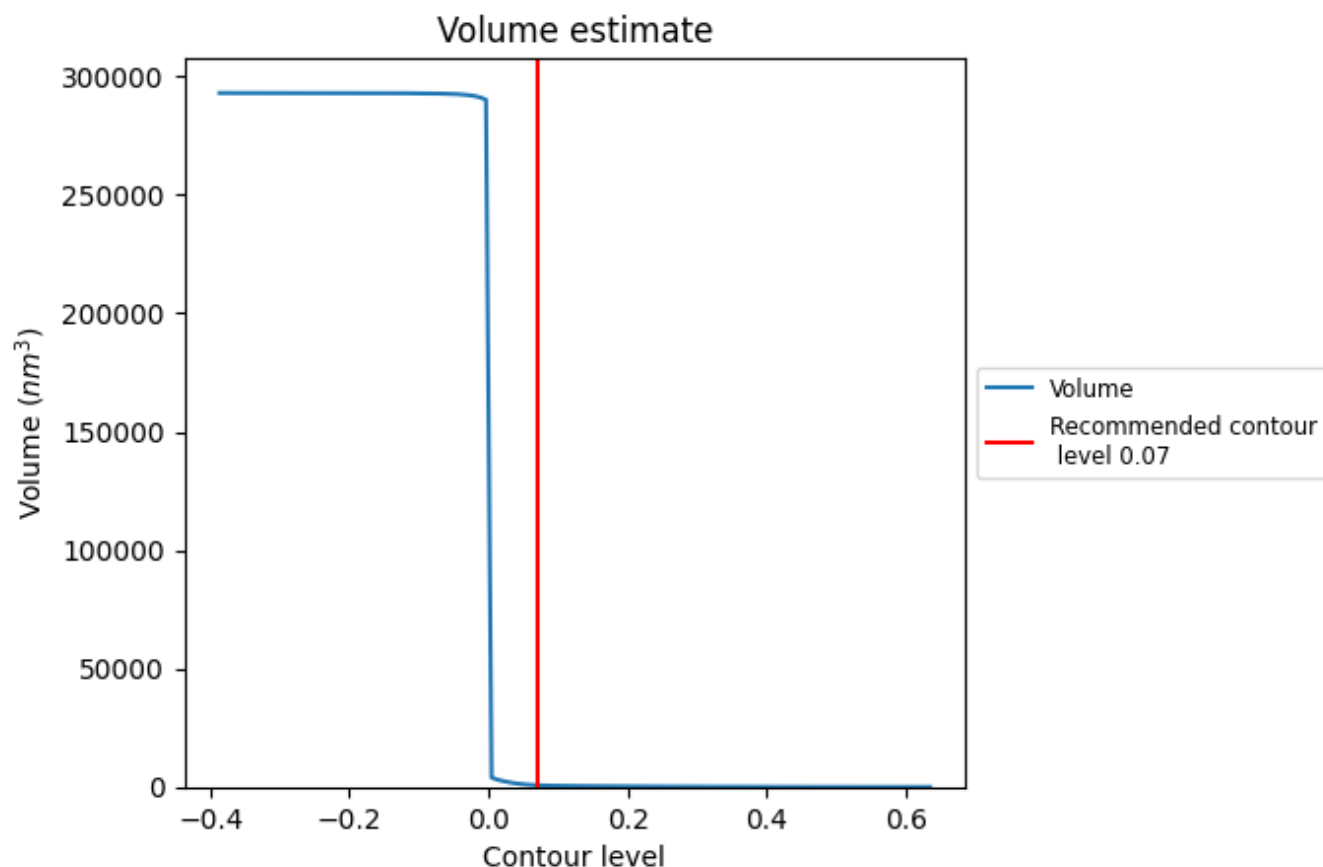
This section contains the results of statistical analysis of the map.

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.

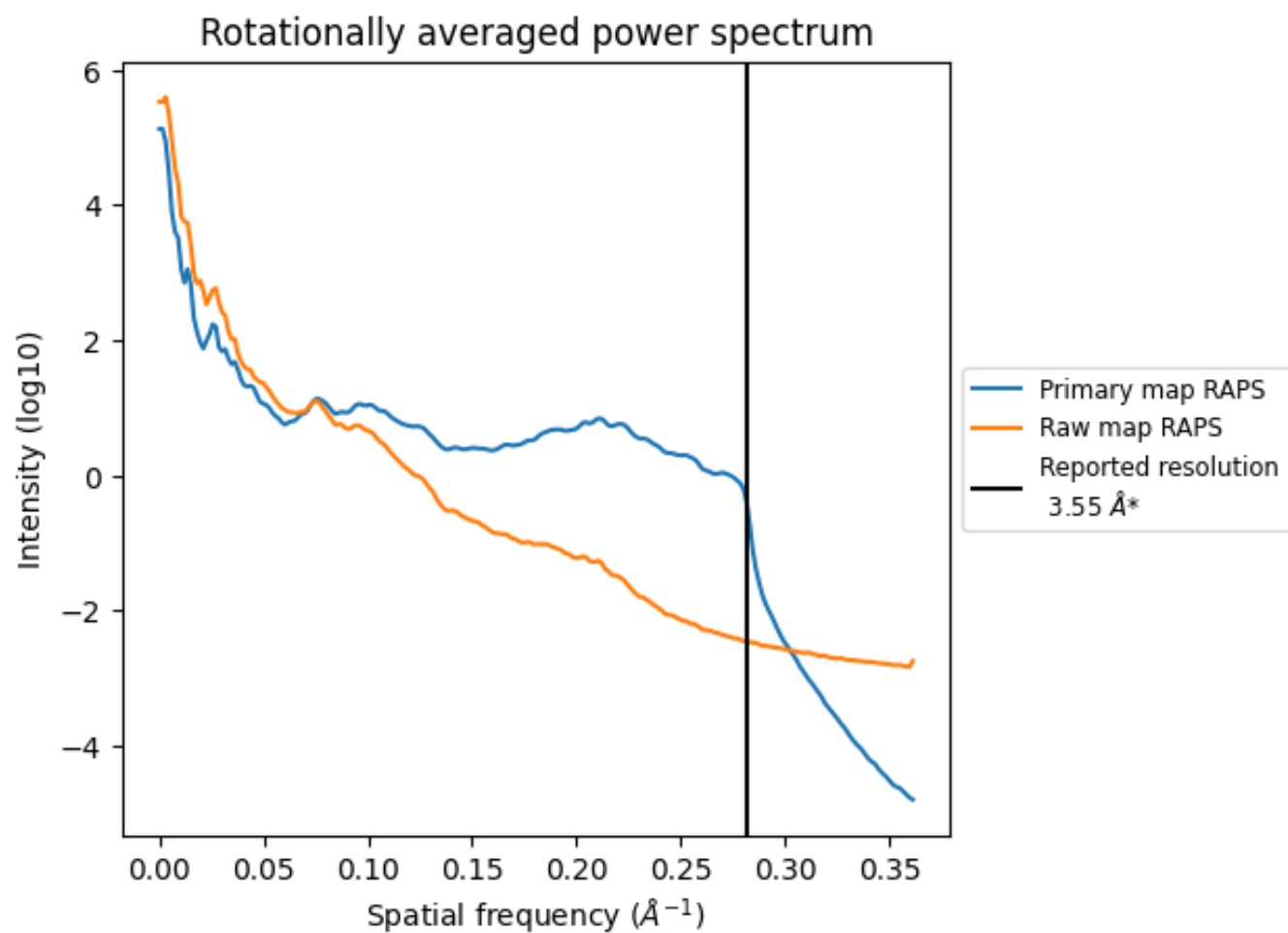
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm³; this corresponds to an approximate mass of 653 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 ⓘ

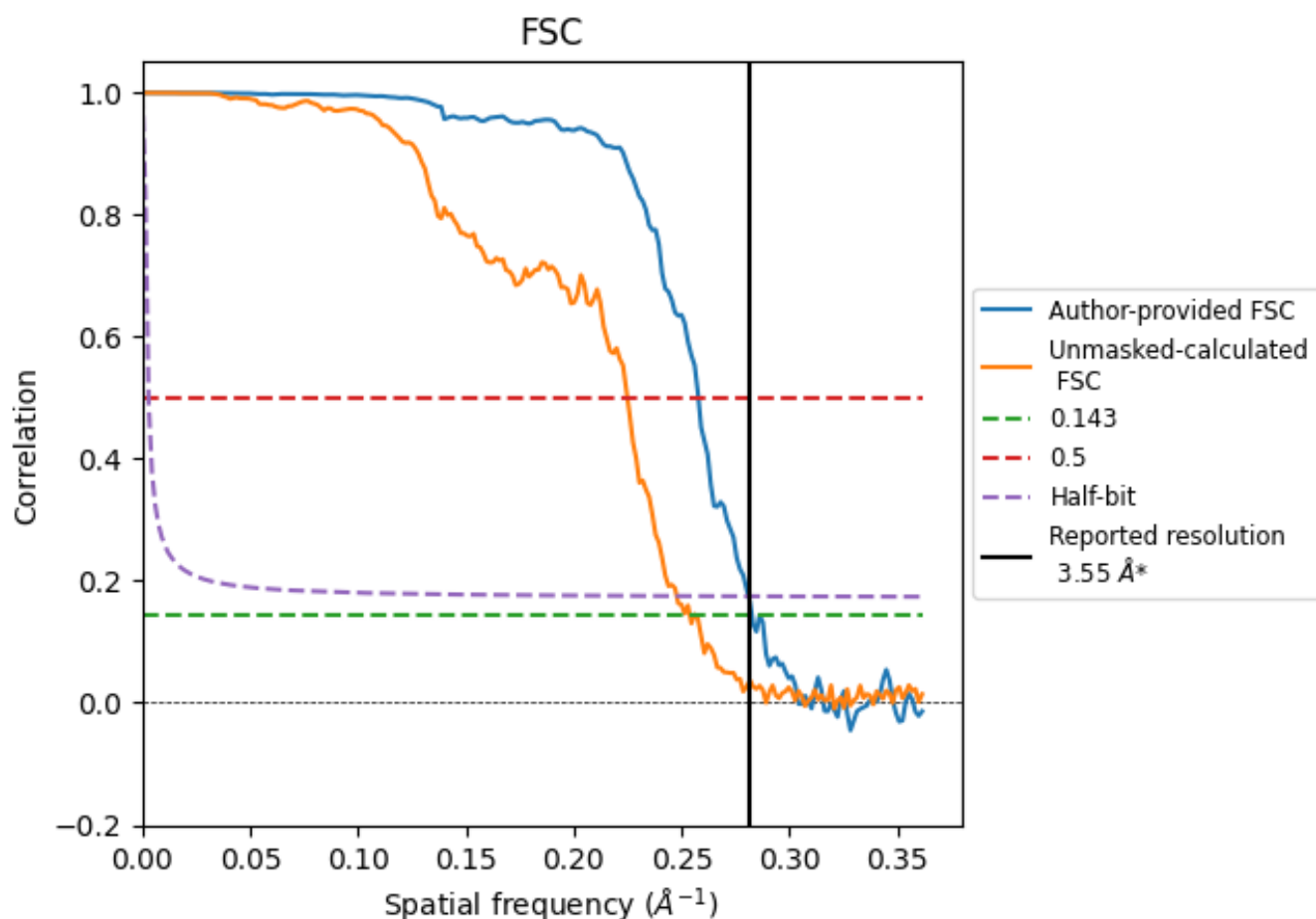


*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

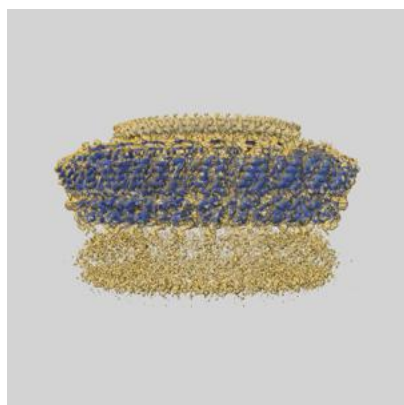
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	3.54	3.88	3.56
Unmasked-calculated*	3.94	4.45	4.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.55 by more than 10 %

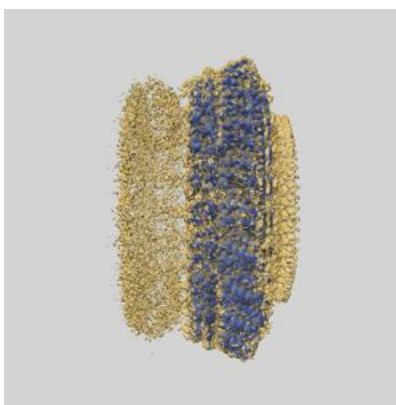
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10045 and PDB model 6RWX. Per-residue inclusion information can be found in section [3](#) on page [8](#).

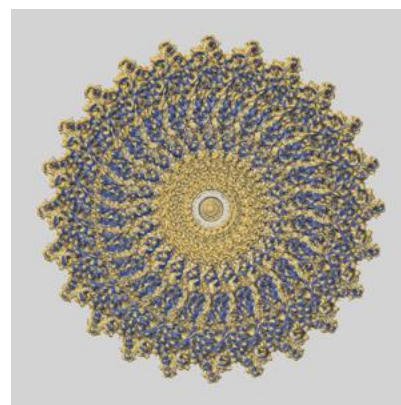
9.1 Map-model overlay [i](#)



X



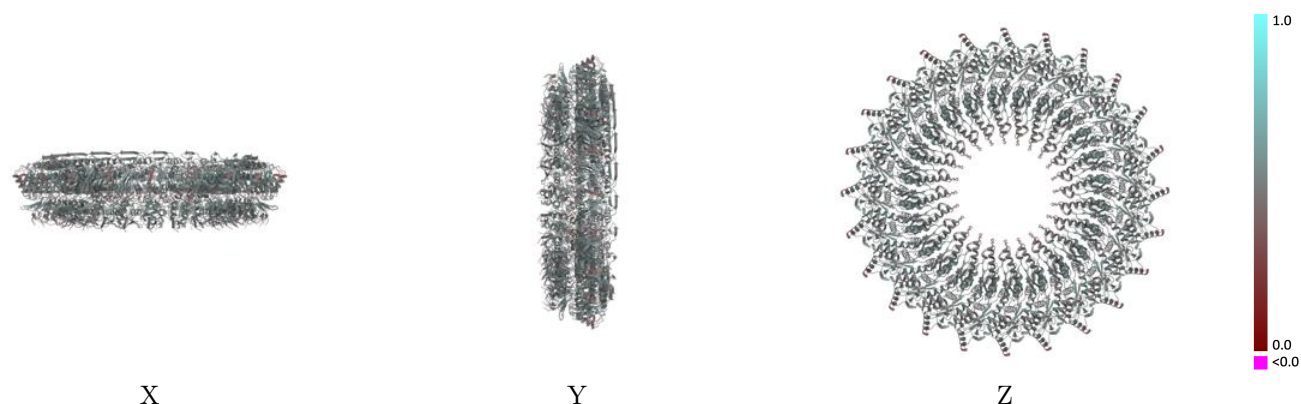
Y



Z

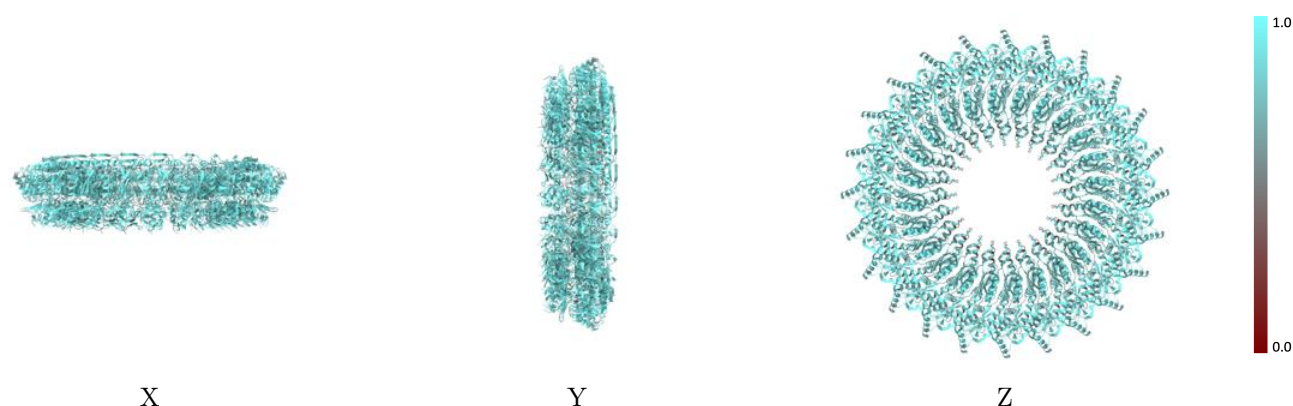
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



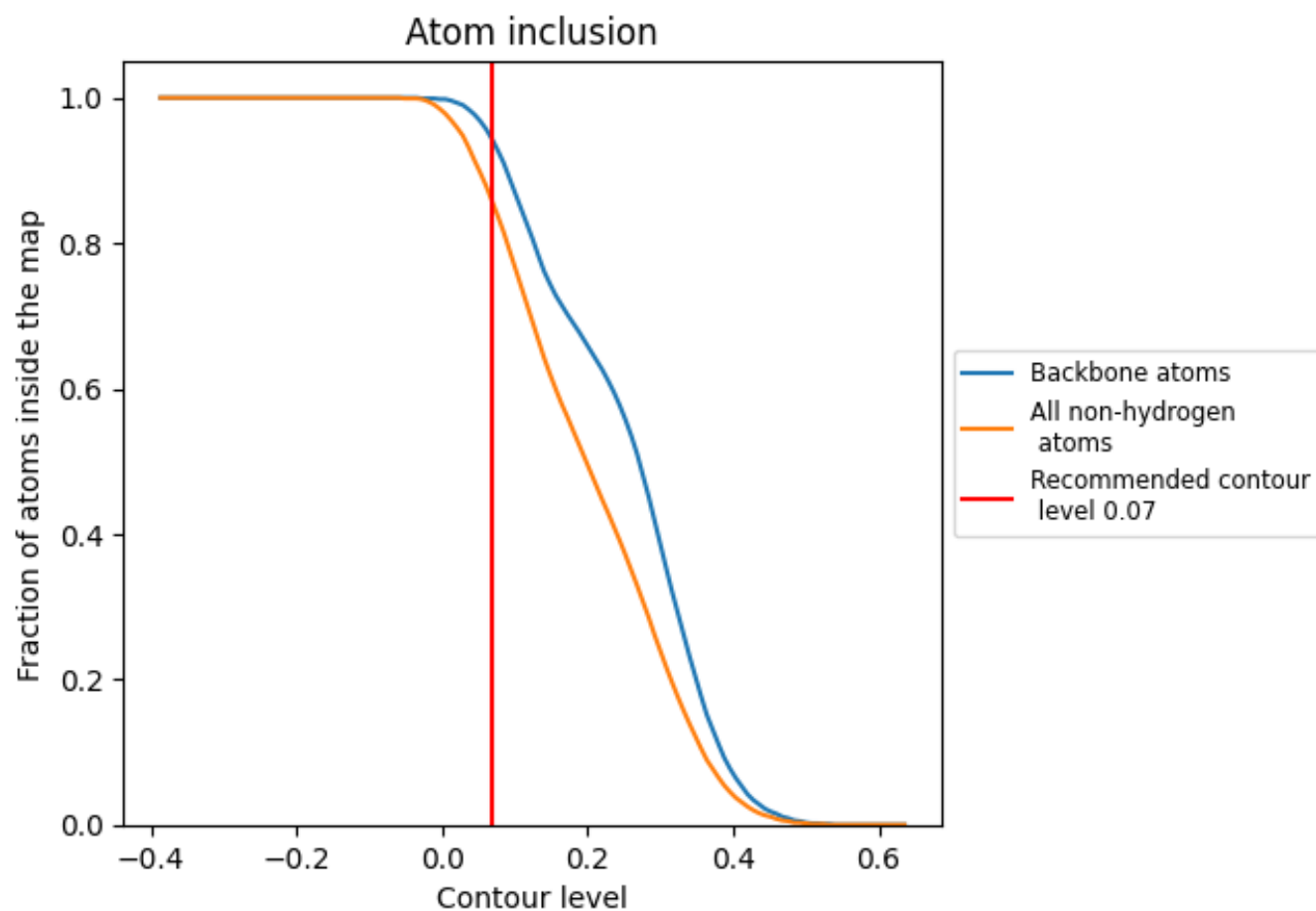
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.4920
A	 0.8810	 0.4990
B	 0.8810	 0.5020
C	 0.8860	 0.5020
D	 0.8680	 0.4910
E	 0.8730	 0.4920
F	 0.8740	 0.4940
G	 0.8660	 0.4890
H	 0.8720	 0.4970
I	 0.8690	 0.4950
J	 0.8780	 0.4980
K	 0.8770	 0.4970
L	 0.8840	 0.5020
M	 0.8790	 0.5000
N	 0.8770	 0.5030
O	 0.8830	 0.5020
P	 0.8820	 0.5030
Q	 0.8750	 0.5010
R	 0.8670	 0.4930
S	 0.8680	 0.4940
T	 0.8690	 0.4940
U	 0.8680	 0.4960
V	 0.8770	 0.5030
W	 0.8850	 0.5020
X	 0.8610	 0.4920
a	 0.8360	 0.4870
b	 0.8180	 0.4760
c	 0.8370	 0.4860
d	 0.8320	 0.4750
e	 0.8240	 0.4780
f	 0.8260	 0.4840
g	 0.8280	 0.4850
h	 0.8380	 0.4870
i	 0.8370	 0.4900
j	 0.8390	 0.4850



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Chain	Atom inclusion	Q-score
k	 0.8420	 0.4900
l	 0.8360	 0.4870
m	 0.8360	 0.4850
n	 0.8340	 0.4870
o	 0.8370	 0.4890
p	 0.8380	 0.4860
q	 0.8420	 0.4910
r	 0.8350	 0.4920
s	 0.8290	 0.4810
t	 0.8390	 0.4860
u	 0.8340	 0.4900
v	 0.8330	 0.4840
w	 0.8340	 0.4810
x	 0.8310	 0.4850