



## Full wwPDB EM Validation Report ⓘ

Apr 14, 2025 – 04:20 PM JST

PDB ID : 7CLR / pdb\_00007clr  
EMDB ID : EMD-30398  
Title : CryoEM structure of S.typhimurium flagellar LP ring  
Authors : Yamaguchi, T.; Makino, F.; Miyata, T.; Minamino, T.; Kato, T.; Namba, K.  
Deposited on : 2020-07-21  
Resolution : 3.50 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](mailto: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.dev117  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

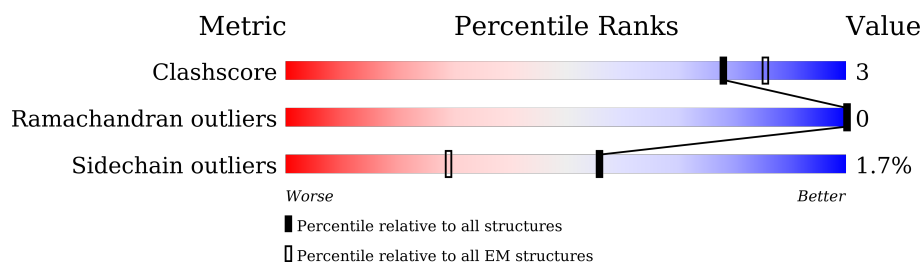
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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




























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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	232	85% 6% 9%
1	B	232	86% 5% 9%
1	C	232	86% 5% 9%
1	D	232	86% 5% 9%
1	E	232	85% 6% 9%
1	F	232	85% 6% 9%
1	G	232	84% 6% 9%
1	H	232	85% 6% 9%
1	I	232	85% 6% 9%



















*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	J	232	
1	K	232	
1	L	232	
1	M	232	
1	N	232	
1	O	232	
1	P	232	
1	Q	232	
1	R	232	
1	S	232	
1	T	232	
1	U	232	
1	V	232	
1	W	232	
1	X	232	
1	Y	232	
1	Z	232	
2	a	365	
2	b	365	
2	c	365	
2	d	365	
2	e	365	
2	f	365	
2	g	365	
2	h	365	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	i	365	 82% 17%
2	j	365	 82% 17%
2	k	365	 82% 17%
2	l	365	 82% 17%
2	m	365	 82% 17%
2	n	365	 82% 17%
2	o	365	 82% 17%
2	p	365	 82% 17%
2	q	365	 82% 17%
2	r	365	 82% 17%
2	s	365	 82% 17%
2	t	365	 82% 17%
2	u	365	 82% 17%
2	v	365	 82% 17%
2	w	365	 82% 17%
2	x	365	 82% 17%
2	y	365	 82% 17%
2	z	365	 82% 17%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 99008 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 Flagellar L-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	B	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	C	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	D	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	E	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	F	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	G	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	H	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	I	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	J	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	K	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	L	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	M	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	N	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	O	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	P	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	Q	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	S	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	T	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	U	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	V	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	W	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	X	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	Y	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		
1	Z	211	Total	C	N	O	S	0	0
			1580	985	282	309	4		

- Molecule 2 is a protein called Flagellar P-ring protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	b	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	c	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	d	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	e	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	f	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	g	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	h	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	i	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	j	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		

*Continued on next page...*


*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	l	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	m	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	n	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	o	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	p	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	q	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	r	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	s	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	t	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	u	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	v	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	w	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	x	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	y	303	Total 2228	C 1364	N 405	O 446	S 13	0	0
2	z	303	Total 2228	C 1364	N 405	O 446	S 13	0	0

### 3 Residue-property plots [i](#)


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

- Molecule 1: Flagellar L-ring protein

Chain A: 



- Molecule 1: Flagellar L-ring protein

Chain B: 



- Molecule 1: Flagellar L-ring protein

Chain C: 




- Molecule 1: Flagellar L-ring protein

Chain D: 




- Molecule 1: Flagellar L-ring protein

Chain E: 



- Molecule 1: Flagellar L-ring protein

Chain F: 





- Molecule 1: Flagellar L-ring protein

Chain G: 84% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain H: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain I: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain J: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain K: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain L: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain M: 85% 6% 9%



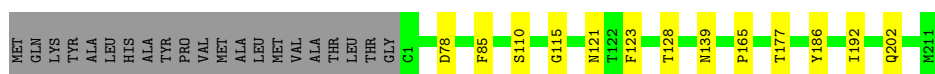
- Molecule 1: Flagellar L-ring protein

Chain N: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain O: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain P: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain Q: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain R: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain S: 85% 6% 9%



- Molecule 1: Flagellar L-ring protein

Chain T: 84% 6% 9%



- Molecule 1: Flagellar L-ring protein



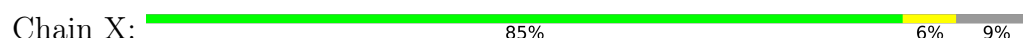
- Molecule 1: Flagellar L-ring protein



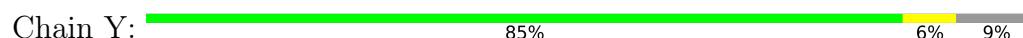
- Molecule 1: Flagellar L-ring protein



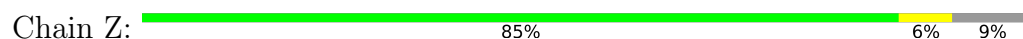
- Molecule 1: Flagellar L-ring protein



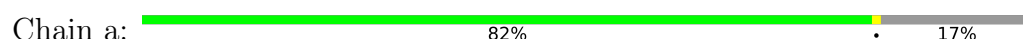
- Molecule 1: Flagellar L-ring protein

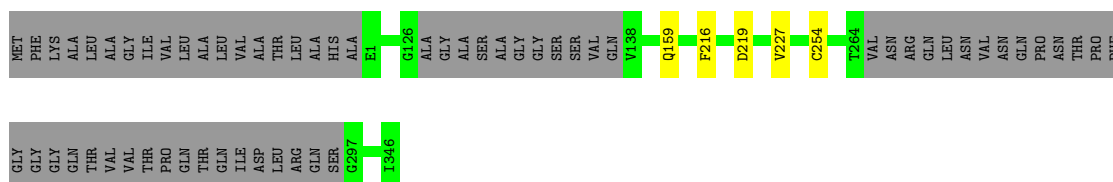


- Molecule 1: Flagellar L-ring protein

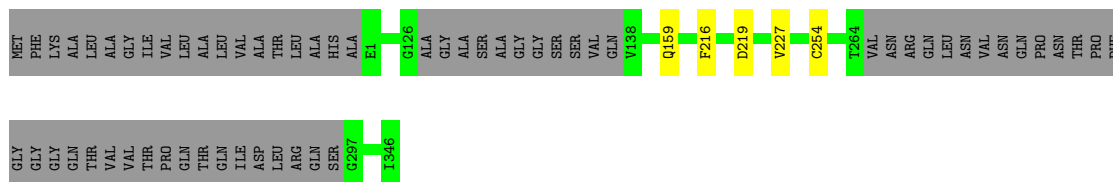
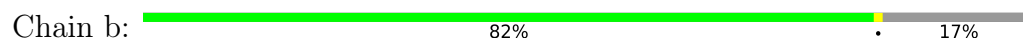


- Molecule 2: Flagellar P-ring protein

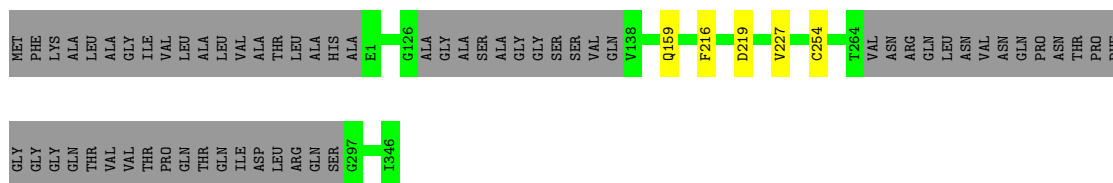
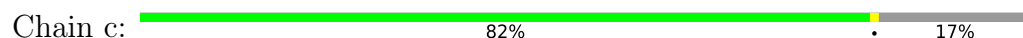




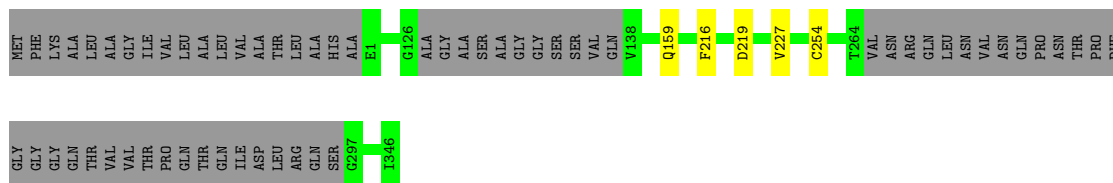
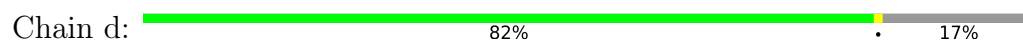
- Molecule 2: Flagellar P-ring protein



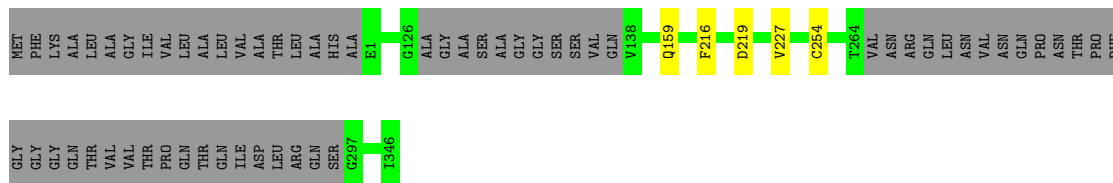
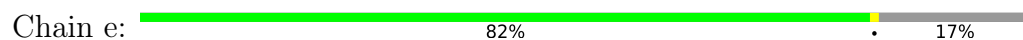
- Molecule 2: Flagellar P-ring protein



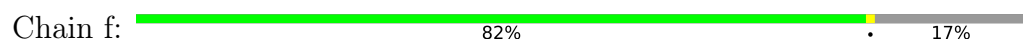
- Molecule 2: Flagellar P-ring protein

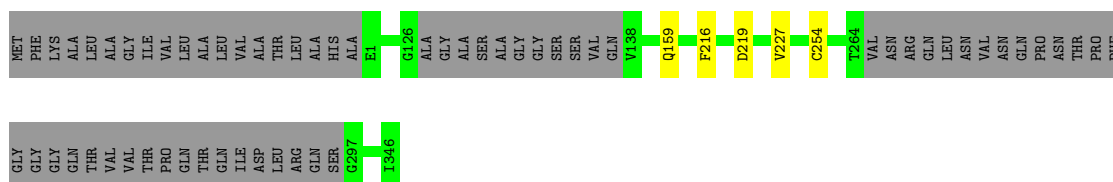


- Molecule 2: Flagellar P-ring protein



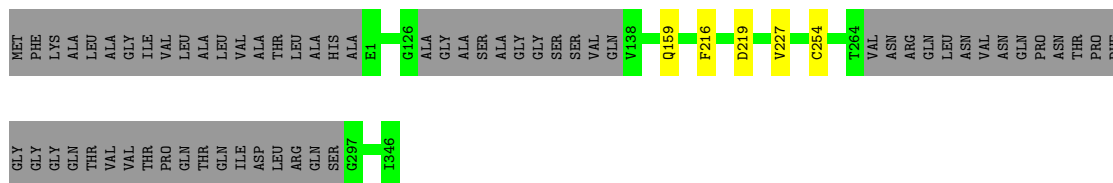
- Molecule 2: Flagellar P-ring protein





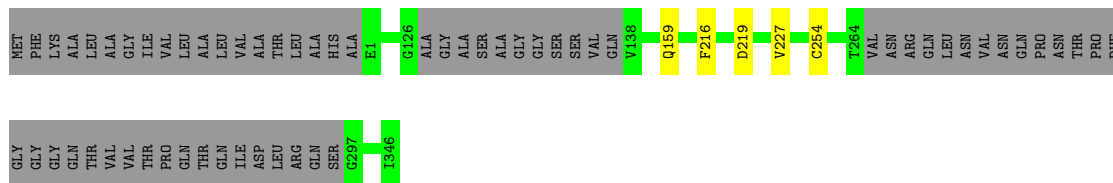
- Molecule 2: Flagellar P-ring protein

Chain g: 82% 17%



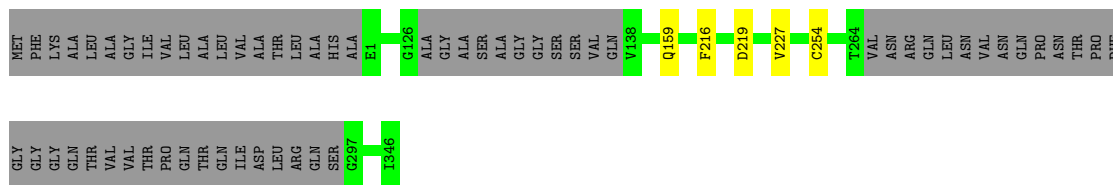
- Molecule 2: Flagellar P-ring protein

Chain h: 82% 17%



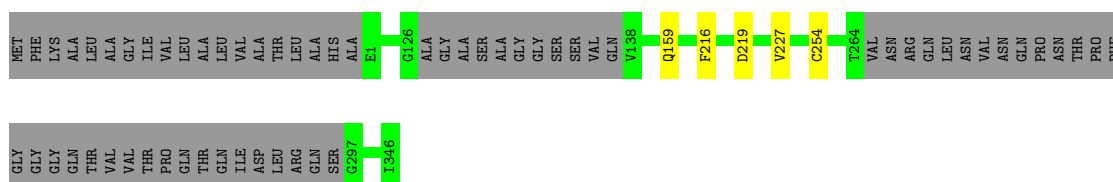
- Molecule 2: Flagellar P-ring protein

Chain i: 82% 17%




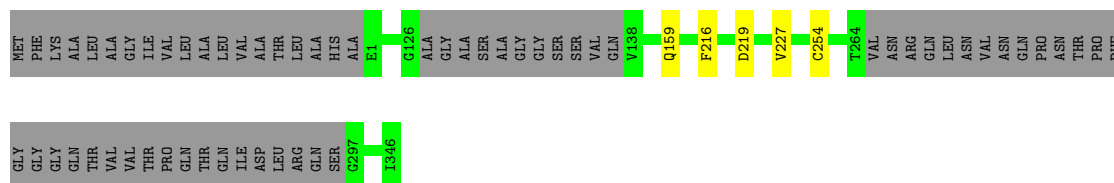
- Molecule 2: Flagellar P-ring protein

Chain j: 82% 17%




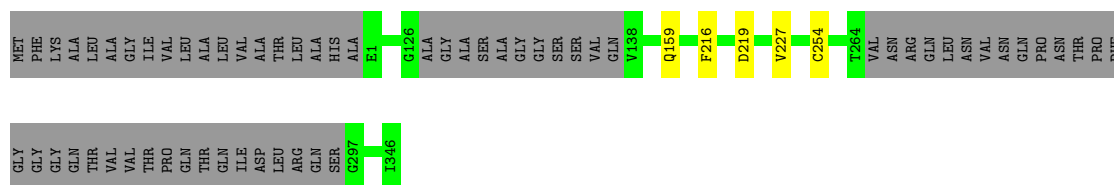
- Molecule 2: Flagellar P-ring protein

Chain k:  82% 17%




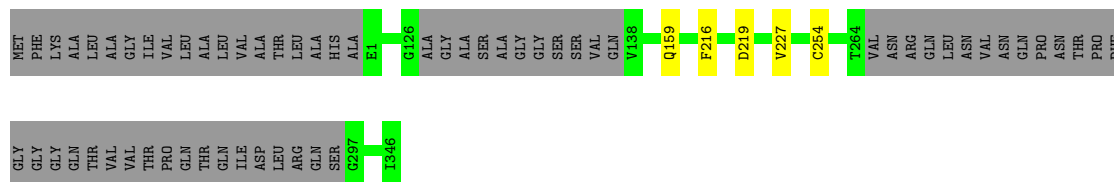
- Molecule 2: Flagellar P-ring protein

Chain l:  82% 17%




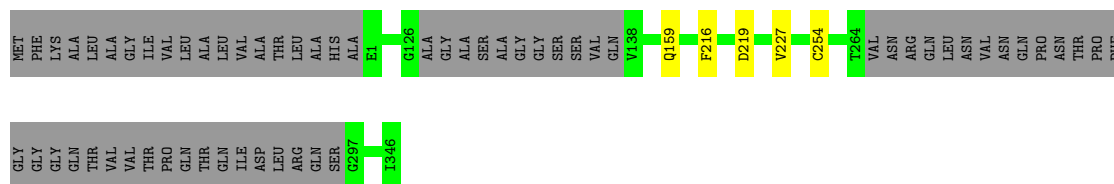
- Molecule 2: Flagellar P-ring protein

Chain m:  82% 17%




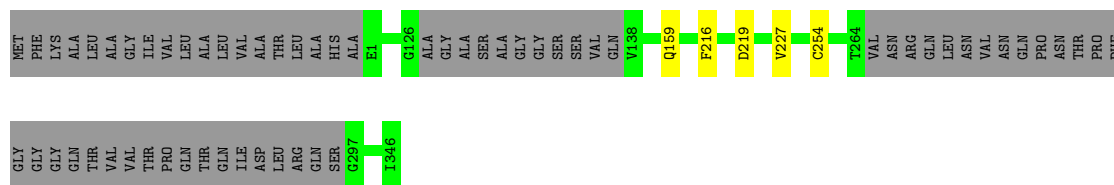
- Molecule 2: Flagellar P-ring protein

Chain n:  82% 17%




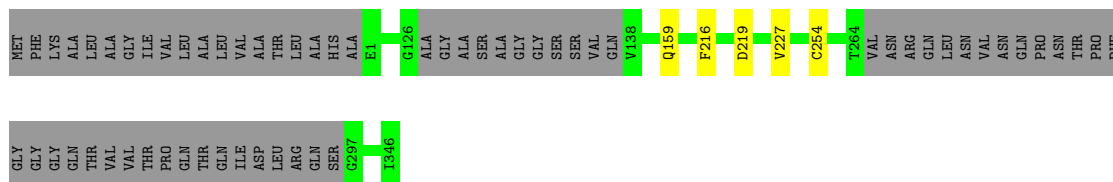
- Molecule 2: Flagellar P-ring protein

Chain o:  82% 17%




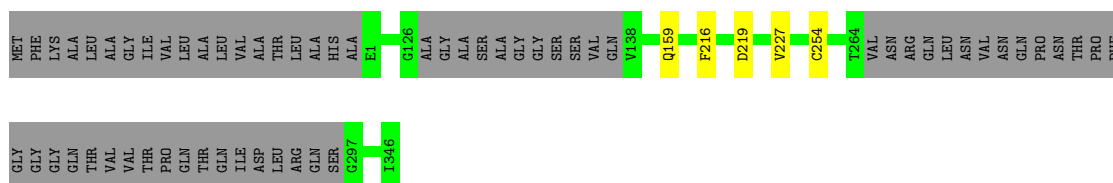
- Molecule 2: Flagellar P-ring protein

Chain p:  82% 17%




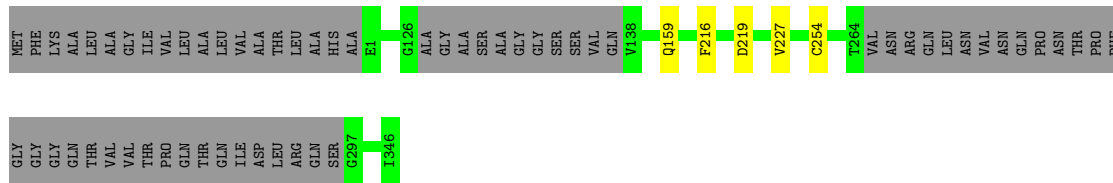
• Molecule 2: Flagellar P-ring protein

Chain q:  82% 17%




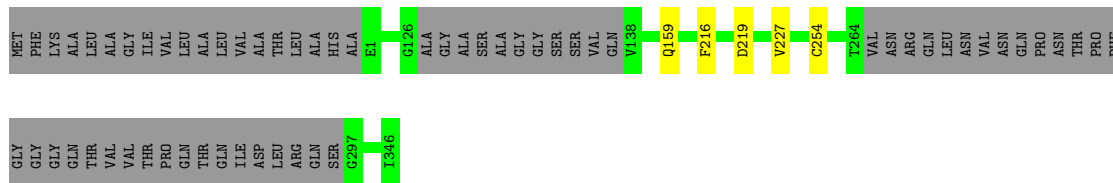
• Molecule 2: Flagellar P-ring protein

Chain r:  82% 17%




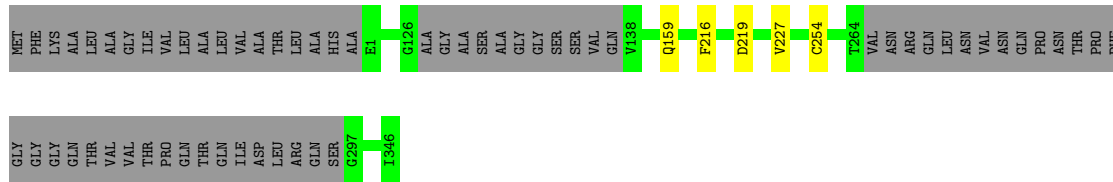
• Molecule 2: Flagellar P-ring protein

Chain s:  82% 17%




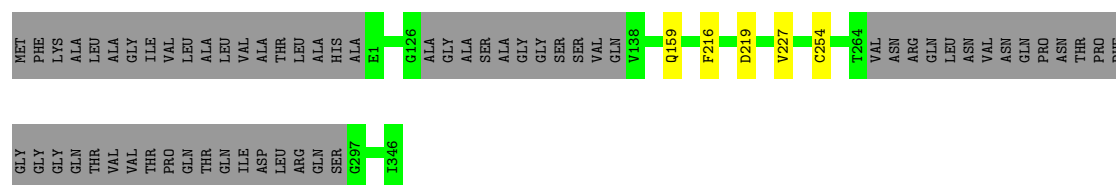
• Molecule 2: Flagellar P-ring protein

Chain t:  82% 17%




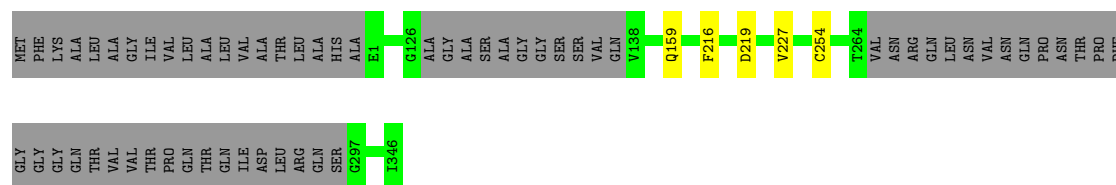
• Molecule 2: Flagellar P-ring protein

Chain u:  82% 17%




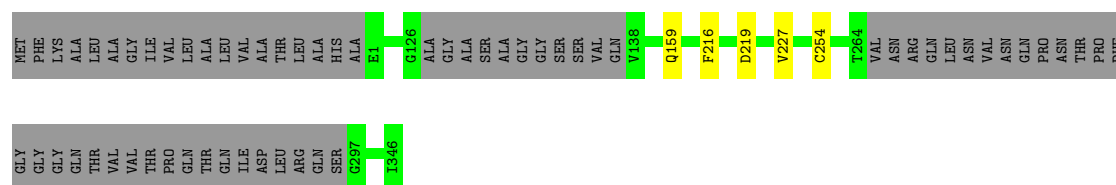
• Molecule 2: Flagellar P-ring protein

Chain v:  82% 17%




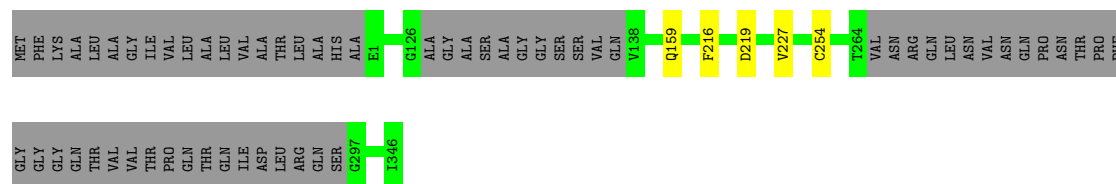
• Molecule 2: Flagellar P-ring protein

Chain w:  82% 17%




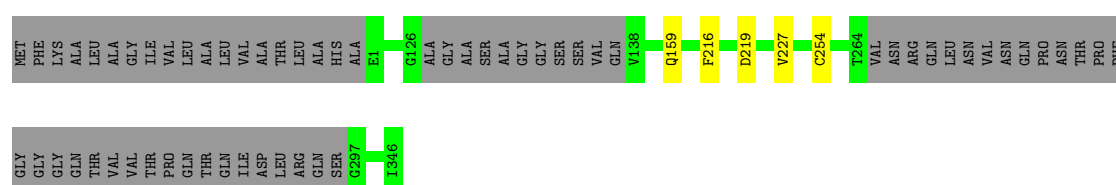
• Molecule 2: Flagellar P-ring protein

Chain x:  82% 17%



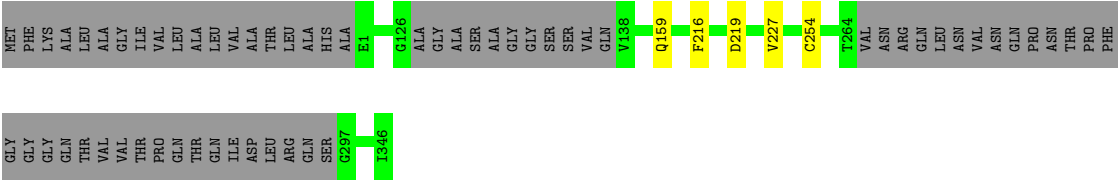
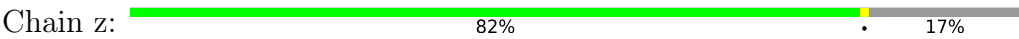
• Molecule 2: Flagellar P-ring protein

Chain y:  82% 17%



• Molecule 2: Flagellar P-ring protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C26	Depositor
Number of particles used	10802	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	275	Depositor
Maximum defocus (nm)	8230	Depositor
Magnification	40000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	0.27	0/1613	0.51	0/2194
1	B	0.26	0/1613	0.52	0/2194
1	C	0.27	0/1613	0.52	0/2194
1	D	0.27	0/1613	0.51	0/2194
1	E	0.27	0/1613	0.52	0/2194
1	F	0.26	0/1613	0.52	0/2194
1	G	0.27	0/1613	0.52	0/2194
1	H	0.27	0/1613	0.51	0/2194
1	I	0.26	0/1613	0.52	0/2194
1	J	0.27	0/1613	0.51	0/2194
1	K	0.27	0/1613	0.51	0/2194
1	L	0.27	0/1613	0.51	0/2194
1	M	0.27	0/1613	0.52	0/2194
1	N	0.27	0/1613	0.52	0/2194
1	O	0.26	0/1613	0.51	0/2194
1	P	0.27	0/1613	0.52	0/2194
1	Q	0.26	0/1613	0.52	0/2194
1	R	0.27	0/1613	0.52	0/2194
1	S	0.27	0/1613	0.51	0/2194
1	T	0.27	0/1613	0.51	0/2194
1	U	0.26	0/1613	0.52	0/2194
1	V	0.26	0/1613	0.51	0/2194
1	W	0.26	0/1613	0.52	0/2194
1	X	0.27	0/1613	0.52	0/2194
1	Y	0.26	0/1613	0.52	0/2194
1	Z	0.26	0/1613	0.52	0/2194
2	a	0.24	0/2243	0.49	0/3041
2	b	0.25	0/2243	0.49	0/3041
2	c	0.24	0/2243	0.49	0/3041
2	d	0.24	0/2243	0.49	0/3041
2	e	0.24	0/2243	0.49	0/3041
2	f	0.25	0/2243	0.49	0/3041
2	g	0.25	0/2243	0.50	0/3041
2	h	0.24	0/2243	0.49	0/3041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	i	0.25	0/2243	0.49	0/3041
2	j	0.25	0/2243	0.49	0/3041
2	k	0.24	0/2243	0.49	0/3041
2	l	0.24	0/2243	0.49	0/3041
2	m	0.25	0/2243	0.49	0/3041
2	n	0.24	0/2243	0.49	0/3041
2	o	0.24	0/2243	0.50	0/3041
2	p	0.24	0/2243	0.49	0/3041
2	q	0.25	0/2243	0.49	0/3041
2	r	0.24	0/2243	0.49	0/3041
2	s	0.25	0/2243	0.50	0/3041
2	t	0.25	0/2243	0.49	0/3041
2	u	0.24	0/2243	0.49	0/3041
2	v	0.24	0/2243	0.49	0/3041
2	w	0.24	0/2243	0.49	0/3041
2	x	0.24	0/2243	0.49	0/3041
2	y	0.24	0/2243	0.49	0/3041
2	z	0.25	0/2243	0.49	0/3041
All	All	0.25	0/100256	0.50	0/136110

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1580	0	1537	10	0
1	B	1580	0	1537	9	0
1	C	1580	0	1537	9	0
1	D	1580	0	1537	9	0
1	E	1580	0	1537	10	0
1	F	1580	0	1537	10	0
1	G	1580	0	1537	12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1580	0	1537	10	0
1	I	1580	0	1537	11	0
1	J	1580	0	1537	10	0
1	K	1580	0	1537	10	0
1	L	1580	0	1537	10	0
1	M	1580	0	1537	11	0
1	N	1580	0	1537	11	0
1	O	1580	0	1537	10	0
1	P	1580	0	1537	10	0
1	Q	1580	0	1537	10	0
1	R	1580	0	1537	10	0
1	S	1580	0	1537	11	0
1	T	1580	0	1537	12	0
1	U	1580	0	1537	11	0
1	V	1580	0	1537	10	0
1	W	1580	0	1537	10	0
1	X	1580	0	1537	10	0
1	Y	1580	0	1537	11	0
1	Z	1580	0	1537	11	0
2	a	2228	0	2268	0	0
2	b	2228	0	2268	0	0
2	c	2228	0	2268	0	0
2	d	2228	0	2268	0	0
2	e	2228	0	2268	0	0
2	f	2228	0	2268	0	0
2	g	2228	0	2268	0	0
2	h	2228	0	2268	0	0
2	i	2228	0	2268	0	0
2	j	2228	0	2268	0	0
2	k	2228	0	2268	0	0
2	l	2228	0	2268	0	0
2	m	2228	0	2268	0	0
2	n	2228	0	2268	0	0
2	o	2228	0	2268	0	0
2	p	2228	0	2268	0	0
2	q	2228	0	2268	0	0
2	r	2228	0	2268	0	0
2	s	2228	0	2268	0	0
2	t	2228	0	2268	0	0
2	u	2228	0	2268	0	0
2	v	2228	0	2268	0	0
2	w	2228	0	2268	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	x	2228	0	2268	0	0
2	y	2228	0	2268	0	0
2	z	2228	0	2268	0	0
All	All	99008	0	98930	160	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 (160) 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:K:121:ASN:ND2	1:L:186:TYR:OH	2.43	0.52
1:A:177:THR:O	1:B:128:THR:OG1	2.28	0.52
1:L:121:ASN:ND2	1:M:186:TYR:OH	2.43	0.52
1:I:121:ASN:ND2	1:J:186:TYR:OH	2.44	0.51
1:J:121:ASN:ND2	1:K:186:TYR:OH	2.44	0.51
1:T:177:THR:O	1:U:128:THR:OG1	2.28	0.51
1:V:121:ASN:ND2	1:W:186:TYR:OH	2.43	0.51
1:X:121:ASN:ND2	1:Y:186:TYR:OH	2.43	0.51
1:B:177:THR:O	1:C:128:THR:OG1	2.29	0.51
1:Y:177:THR:O	1:Z:128:THR:OG1	2.29	0.50
1:F:177:THR:O	1:G:128:THR:OG1	2.29	0.50
1:H:177:THR:O	1:I:128:THR:OG1	2.29	0.50
1:T:121:ASN:ND2	1:U:186:TYR:OH	2.44	0.50
1:Y:121:ASN:ND2	1:Z:186:TYR:OH	2.43	0.50
1:X:177:THR:O	1:Y:128:THR:OG1	2.30	0.50
1:C:121:ASN:ND2	1:D:186:TYR:OH	2.43	0.50
1:W:121:ASN:ND2	1:X:186:TYR:OH	2.44	0.50
1:M:177:THR:O	1:N:128:THR:OG1	2.29	0.50
1:S:121:ASN:ND2	1:T:186:TYR:OH	2.44	0.50
1:A:128:THR:OG1	1:Z:177:THR:O	2.29	0.49
1:N:177:THR:O	1:O:128:THR:OG1	2.30	0.49
1:A:121:ASN:ND2	1:B:186:TYR:OH	2.43	0.49
1:O:177:THR:O	1:P:128:THR:OG1	2.29	0.49
1:B:121:ASN:ND2	1:C:186:TYR:OH	2.44	0.49
1:U:121:ASN:ND2	1:V:186:TYR:OH	2.45	0.49
1:V:177:THR:O	1:W:128:THR:OG1	2.30	0.49
1:G:177:THR:O	1:H:128:THR:OG1	2.30	0.49
1:S:177:THR:O	1:T:128:THR:OG1	2.29	0.49
1:D:121:ASN:ND2	1:E:186:TYR:OH	2.44	0.49
1:E:177:THR:O	1:F:128:THR:OG1	2.31	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:THR:O	1:D:128:THR:OG1	2.30	0.49
1:D:177:THR:O	1:E:128:THR:OG1	2.30	0.49
1:Q:121:ASN:ND2	1:R:186:TYR:OH	2.44	0.49
1:R:121:ASN:ND2	1:S:186:TYR:OH	2.44	0.49
1:A:186:TYR:OH	1:Z:121:ASN:ND2	2.44	0.49
1:L:177:THR:O	1:M:128:THR:OG1	2.29	0.49
1:U:177:THR:O	1:V:128:THR:OG1	2.31	0.49
1:I:177:THR:O	1:J:128:THR:OG1	2.30	0.48
1:P:177:THR:O	1:Q:128:THR:OG1	2.30	0.48
1:Q:177:THR:O	1:R:128:THR:OG1	2.30	0.48
1:R:177:THR:O	1:S:128:THR:OG1	2.30	0.48
1:J:177:THR:O	1:K:128:THR:OG1	2.30	0.48
1:W:177:THR:O	1:X:128:THR:OG1	2.31	0.48
1:E:121:ASN:ND2	1:F:186:TYR:OH	2.44	0.48
1:K:177:THR:O	1:L:128:THR:OG1	2.31	0.48
1:P:121:ASN:ND2	1:Q:186:TYR:OH	2.43	0.48
1:F:121:ASN:ND2	1:G:186:TYR:OH	2.45	0.47
1:M:121:ASN:ND2	1:N:186:TYR:OH	2.44	0.47
1:J:139:ASN:HA	1:J:165:PRO:HD3	1.97	0.47
1:U:139:ASN:HA	1:U:165:PRO:HD3	1.97	0.47
1:V:139:ASN:HA	1:V:165:PRO:HD3	1.97	0.47
1:E:139:ASN:HA	1:E:165:PRO:HD3	1.97	0.47
1:K:139:ASN:HA	1:K:165:PRO:HD3	1.97	0.47
1:L:139:ASN:HA	1:L:165:PRO:HD3	1.97	0.47
1:P:139:ASN:HA	1:P:165:PRO:HD3	1.97	0.47
1:H:121:ASN:ND2	1:I:186:TYR:OH	2.44	0.46
1:N:121:ASN:ND2	1:O:186:TYR:OH	2.44	0.46
1:T:139:ASN:HA	1:T:165:PRO:HD3	1.97	0.46
1:G:121:ASN:ND2	1:H:186:TYR:OH	2.44	0.46
1:W:139:ASN:HA	1:W:165:PRO:HD3	1.97	0.46
1:C:139:ASN:HA	1:C:165:PRO:HD3	1.97	0.46
1:D:139:ASN:HA	1:D:165:PRO:HD3	1.97	0.46
1:B:139:ASN:HA	1:B:165:PRO:HD3	1.97	0.46
1:O:139:ASN:HA	1:O:165:PRO:HD3	1.97	0.46
1:F:139:ASN:HA	1:F:165:PRO:HD3	1.97	0.46
1:I:139:ASN:HA	1:I:165:PRO:HD3	1.97	0.46
1:Q:139:ASN:HA	1:Q:165:PRO:HD3	1.97	0.46
1:X:139:ASN:HA	1:X:165:PRO:HD3	1.97	0.46
1:A:139:ASN:HA	1:A:165:PRO:HD3	1.97	0.46
1:O:121:ASN:ND2	1:P:186:TYR:OH	2.45	0.46
1:G:139:ASN:HA	1:G:165:PRO:HD3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:ASN:HA	1:H:165:PRO:HD3	1.97	0.46
1:R:139:ASN:HA	1:R:165:PRO:HD3	1.97	0.46
1:M:139:ASN:HA	1:M:165:PRO:HD3	1.97	0.45
1:N:139:ASN:HA	1:N:165:PRO:HD3	1.97	0.45
1:Z:139:ASN:HA	1:Z:165:PRO:HD3	1.97	0.45
1:S:139:ASN:HA	1:S:165:PRO:HD3	1.97	0.45
1:Y:139:ASN:HA	1:Y:165:PRO:HD3	1.97	0.45
1:H:78:ASP:N	1:H:78:ASP:OD1	2.51	0.45
1:M:78:ASP:N	1:M:78:ASP:OD1	2.51	0.44
1:Q:78:ASP:OD1	1:Q:78:ASP:N	2.51	0.44
1:S:78:ASP:OD1	1:S:78:ASP:N	2.51	0.44
1:T:78:ASP:N	1:T:78:ASP:OD1	2.51	0.44
1:I:78:ASP:OD1	1:I:78:ASP:N	2.51	0.44
1:N:78:ASP:OD1	1:N:78:ASP:N	2.51	0.44
1:R:78:ASP:OD1	1:R:78:ASP:N	2.51	0.44
1:U:78:ASP:OD1	1:U:78:ASP:N	2.51	0.44
1:Y:78:ASP:N	1:Y:78:ASP:OD1	2.51	0.44
1:C:78:ASP:N	1:C:78:ASP:OD1	2.51	0.44
1:G:78:ASP:OD1	1:G:78:ASP:N	2.51	0.44
1:S:115:GLY:HA3	1:U:192:ILE:HG23	2.00	0.44
1:X:78:ASP:OD1	1:X:78:ASP:N	2.51	0.44
1:A:78:ASP:OD1	1:A:78:ASP:N	2.51	0.44
1:B:78:ASP:OD1	1:B:78:ASP:N	2.51	0.44
1:K:78:ASP:OD1	1:K:78:ASP:N	2.51	0.44
1:L:78:ASP:OD1	1:L:78:ASP:N	2.51	0.44
1:P:78:ASP:OD1	1:P:78:ASP:N	2.51	0.44
1:D:78:ASP:OD1	1:D:78:ASP:N	2.51	0.43
1:F:78:ASP:OD1	1:F:78:ASP:N	2.51	0.43
1:W:78:ASP:OD1	1:W:78:ASP:N	2.51	0.43
1:O:78:ASP:N	1:O:78:ASP:OD1	2.51	0.43
1:J:78:ASP:N	1:J:78:ASP:OD1	2.51	0.43
1:T:72:SER:OG	1:U:118:ASN:OD1	2.29	0.43
1:E:78:ASP:N	1:E:78:ASP:OD1	2.51	0.43
1:O:115:GLY:HA3	1:Q:192:ILE:HG23	2.01	0.43
1:V:78:ASP:N	1:V:78:ASP:OD1	2.51	0.43
1:Z:78:ASP:OD1	1:Z:78:ASP:N	2.51	0.43
1:B:110:SER:O	1:D:202:GLN:NE2	2.52	0.43
1:O:110:SER:O	1:Q:202:GLN:NE2	2.51	0.43
1:T:115:GLY:HA3	1:V:192:ILE:HG23	2.01	0.43
1:U:110:SER:O	1:W:202:GLN:NE2	2.52	0.43
1:V:110:SER:O	1:X:202:GLN:NE2	2.51	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:110:SER:O	1:U:202:GLN:NE2	2.52	0.43
1:A:202:GLN:NE2	1:Y:110:SER:O	2.52	0.42
1:F:110:SER:O	1:H:202:GLN:NE2	2.51	0.42
1:N:115:GLY:HA3	1:P:192:ILE:HG23	2.01	0.42
1:P:110:SER:O	1:R:202:GLN:NE2	2.52	0.42
1:A:110:SER:O	1:C:202:GLN:NE2	2.52	0.42
1:F:115:GLY:HA3	1:H:192:ILE:HG23	2.01	0.42
1:M:72:SER:OG	1:N:118:ASN:OD1	2.30	0.42
1:E:110:SER:O	1:G:202:GLN:NE2	2.53	0.42
1:G:115:GLY:HA3	1:I:192:ILE:HG23	2.01	0.42
1:J:110:SER:O	1:L:202:GLN:NE2	2.53	0.42
1:M:115:GLY:HA3	1:O:192:ILE:HG23	2.02	0.42
1:T:110:SER:O	1:V:202:GLN:NE2	2.52	0.42
1:Y:72:SER:OG	1:Z:118:ASN:OD1	2.30	0.42
1:R:115:GLY:HA3	1:T:192:ILE:HG23	2.02	0.42
1:B:202:GLN:NE2	1:Z:110:SER:O	2.53	0.42
1:K:110:SER:O	1:M:202:GLN:NE2	2.53	0.42
1:L:115:GLY:HA3	1:N:192:ILE:HG23	2.02	0.42
1:X:110:SER:O	1:Z:202:GLN:NE2	2.52	0.42
1:D:110:SER:O	1:F:202:GLN:NE2	2.53	0.41
1:R:110:SER:O	1:T:202:GLN:NE2	2.53	0.41
1:Q:110:SER:O	1:S:202:GLN:NE2	2.54	0.41
1:U:115:GLY:HA3	1:W:192:ILE:HG23	2.02	0.41
1:W:110:SER:O	1:Y:202:GLN:NE2	2.51	0.41
1:A:192:ILE:HG23	1:Y:115:GLY:HA3	2.01	0.41
1:A:115:GLY:HA3	1:C:192:ILE:HG23	2.01	0.41
1:G:110:SER:O	1:I:202:GLN:NE2	2.52	0.41
1:N:110:SER:O	1:P:202:GLN:NE2	2.54	0.41
1:C:110:SER:O	1:E:202:GLN:NE2	2.53	0.41
1:M:110:SER:O	1:O:202:GLN:NE2	2.54	0.41
1:P:115:GLY:HA3	1:R:192:ILE:HG23	2.03	0.41
1:S:72:SER:OG	1:T:118:ASN:OD1	2.30	0.41
1:B:192:ILE:HG23	1:Z:115:GLY:HA3	2.01	0.41
1:L:110:SER:O	1:N:202:GLN:NE2	2.53	0.41
1:Q:115:GLY:HA3	1:S:192:ILE:HG23	2.03	0.41
1:V:115:GLY:HA3	1:X:192:ILE:HG23	2.03	0.41
1:H:72:SER:OG	1:I:118:ASN:OD1	2.30	0.41
1:K:115:GLY:HA3	1:M:192:ILE:HG23	2.03	0.41
1:X:115:GLY:HA3	1:Z:192:ILE:HG23	2.02	0.41
1:I:72:SER:OG	1:J:118:ASN:OD1	2.30	0.41
1:G:72:SER:OG	1:H:118:ASN:OD1	2.30	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:115:GLY:HA3	1:Y:192:ILE:HG23	2.03	0.40
1:E:115:GLY:HA3	1:G:192:ILE:HG23	2.02	0.40
1:J:72:SER:OG	1:K:118:ASN:OD1	2.30	0.40
1:D:72:SER:OG	1:E:118:ASN:OD1	2.29	0.40
1:F:72:SER:OG	1:G:118:ASN:OD1	2.30	0.40
1:I:110:SER:O	1:K:202:GLN:NE2	2.54	0.40
1:J:115:GLY:HA3	1:L:192:ILE:HG23	2.04	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	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	B	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	C	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	D	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	E	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	F	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	G	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	H	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	I	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	J	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	K	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	L	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	M	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	N	209/232 (90%)	205 (98%)	4 (2%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	P	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	Q	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	R	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	S	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	T	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	U	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	V	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	W	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	X	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	Y	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
1	Z	209/232 (90%)	205 (98%)	4 (2%)	0	100	100
2	a	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	b	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	c	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	d	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	e	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	f	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	g	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	h	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	i	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	j	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	k	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	l	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	m	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	n	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	o	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	p	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	q	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	r	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	s	297/365 (81%)	295 (99%)	2 (1%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	t	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	u	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	v	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	w	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	x	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	y	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
2	z	297/365 (81%)	295 (99%)	2 (1%)	0	100	100
All	All	13156/15522 (85%)	13000 (99%)	156 (1%)	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	A	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	B	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	C	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	D	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	E	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	F	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	G	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	H	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	I	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	J	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	K	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	L	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	M	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	N	170/186 (91%)	168 (99%)	2 (1%)	67	82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	P	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	Q	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	R	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	S	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	T	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	U	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	V	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	W	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	X	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	Y	170/186 (91%)	168 (99%)	2 (1%)	67	82
1	Z	170/186 (91%)	168 (99%)	2 (1%)	67	82
2	a	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	b	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	c	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	d	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	e	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	f	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	g	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	h	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	i	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	j	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	k	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	l	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	m	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	n	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	o	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	p	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	q	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	r	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	s	248/294 (84%)	243 (98%)	5 (2%)	50	72

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	t	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	u	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	v	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	w	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	x	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	y	248/294 (84%)	243 (98%)	5 (2%)	50	72
2	z	248/294 (84%)	243 (98%)	5 (2%)	50	72
All	All	10868/12480 (87%)	10686 (98%)	182 (2%)	56	75

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	PHE
1	A	123	PHE
1	B	85	PHE
1	B	123	PHE
1	C	85	PHE
1	C	123	PHE
1	D	85	PHE
1	D	123	PHE
1	E	85	PHE
1	E	123	PHE
1	F	85	PHE
1	F	123	PHE
1	G	85	PHE
1	G	123	PHE
1	H	85	PHE
1	H	123	PHE
1	I	85	PHE
1	I	123	PHE
1	J	85	PHE
1	J	123	PHE
1	K	85	PHE
1	K	123	PHE
1	L	85	PHE
1	L	123	PHE
1	M	85	PHE
1	M	123	PHE
1	N	85	PHE
1	N	123	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	O	85	PHE
1	O	123	PHE
1	P	85	PHE
1	P	123	PHE
1	Q	85	PHE
1	Q	123	PHE
1	R	85	PHE
1	R	123	PHE
1	S	85	PHE
1	S	123	PHE
1	T	85	PHE
1	T	123	PHE
1	U	85	PHE
1	U	123	PHE
1	V	85	PHE
1	V	123	PHE
1	W	85	PHE
1	W	123	PHE
1	X	85	PHE
1	X	123	PHE
1	Y	85	PHE
1	Y	123	PHE
1	Z	85	PHE
1	Z	123	PHE
2	a	159	GLN
2	a	216	PHE
2	a	219	ASP
2	a	227	VAL
2	a	254	CYS
2	b	159	GLN
2	b	216	PHE
2	b	219	ASP
2	b	227	VAL
2	b	254	CYS
2	c	159	GLN
2	c	216	PHE
2	c	219	ASP
2	c	227	VAL
2	c	254	CYS
2	d	159	GLN
2	d	216	PHE
2	d	219	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	d	227	VAL
2	d	254	CYS
2	e	159	GLN
2	e	216	PHE
2	e	219	ASP
2	e	227	VAL
2	e	254	CYS
2	f	159	GLN
2	f	216	PHE
2	f	219	ASP
2	f	227	VAL
2	f	254	CYS
2	g	159	GLN
2	g	216	PHE
2	g	219	ASP
2	g	227	VAL
2	g	254	CYS
2	h	159	GLN
2	h	216	PHE
2	h	219	ASP
2	h	227	VAL
2	h	254	CYS
2	i	159	GLN
2	i	216	PHE
2	i	219	ASP
2	i	227	VAL
2	i	254	CYS
2	j	159	GLN
2	j	216	PHE
2	j	219	ASP
2	j	227	VAL
2	j	254	CYS
2	k	159	GLN
2	k	216	PHE
2	k	219	ASP
2	k	227	VAL
2	k	254	CYS
2	l	159	GLN
2	l	216	PHE
2	l	219	ASP
2	l	227	VAL
2	l	254	CYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	m	159	GLN
2	m	216	PHE
2	m	219	ASP
2	m	227	VAL
2	m	254	CYS
2	n	159	GLN
2	n	216	PHE
2	n	219	ASP
2	n	227	VAL
2	n	254	CYS
2	o	159	GLN
2	o	216	PHE
2	o	219	ASP
2	o	227	VAL
2	o	254	CYS
2	p	159	GLN
2	p	216	PHE
2	p	219	ASP
2	p	227	VAL
2	p	254	CYS
2	q	159	GLN
2	q	216	PHE
2	q	219	ASP
2	q	227	VAL
2	q	254	CYS
2	r	159	GLN
2	r	216	PHE
2	r	219	ASP
2	r	227	VAL
2	r	254	CYS
2	s	159	GLN
2	s	216	PHE
2	s	219	ASP
2	s	227	VAL
2	s	254	CYS
2	t	159	GLN
2	t	216	PHE
2	t	219	ASP
2	t	227	VAL
2	t	254	CYS
2	u	159	GLN
2	u	216	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	u	219	ASP
2	u	227	VAL
2	u	254	CYS
2	v	159	GLN
2	v	216	PHE
2	v	219	ASP
2	v	227	VAL
2	v	254	CYS
2	w	159	GLN
2	w	216	PHE
2	w	219	ASP
2	w	227	VAL
2	w	254	CYS
2	x	159	GLN
2	x	216	PHE
2	x	219	ASP
2	x	227	VAL
2	x	254	CYS
2	y	159	GLN
2	y	216	PHE
2	y	219	ASP
2	y	227	VAL
2	y	254	CYS
2	z	159	GLN
2	z	216	PHE
2	z	219	ASP
2	z	227	VAL
2	z	254	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	B	121	ASN
1	C	121	ASN
1	D	121	ASN
1	E	121	ASN
1	F	121	ASN
1	G	121	ASN
1	H	121	ASN
1	I	121	ASN
1	J	121	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	121	ASN
1	L	121	ASN
1	M	121	ASN
1	N	121	ASN
1	O	121	ASN
1	P	121	ASN
1	Q	121	ASN
1	R	121	ASN
1	S	121	ASN
1	T	121	ASN
1	U	121	ASN
1	V	121	ASN
1	W	121	ASN
1	X	121	ASN
1	Y	121	ASN
1	Z	121	ASN
2	a	113	GLN
2	a	159	GLN
2	a	203	GLN
2	a	226	ASN
2	a	331	GLN
2	b	113	GLN
2	b	159	GLN
2	b	203	GLN
2	b	226	ASN
2	b	331	GLN
2	c	113	GLN
2	c	159	GLN
2	c	203	GLN
2	c	226	ASN
2	c	331	GLN
2	d	113	GLN
2	d	159	GLN
2	d	203	GLN
2	d	226	ASN
2	d	331	GLN
2	e	113	GLN
2	e	159	GLN
2	e	203	GLN
2	e	226	ASN
2	e	331	GLN
2	f	113	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	f	159	GLN
2	f	203	GLN
2	f	226	ASN
2	f	331	GLN
2	g	113	GLN
2	g	159	GLN
2	g	203	GLN
2	g	226	ASN
2	g	331	GLN
2	h	113	GLN
2	h	159	GLN
2	h	203	GLN
2	h	226	ASN
2	h	331	GLN
2	i	113	GLN
2	i	159	GLN
2	i	203	GLN
2	i	226	ASN
2	i	331	GLN
2	j	113	GLN
2	j	159	GLN
2	j	203	GLN
2	j	226	ASN
2	j	331	GLN
2	k	113	GLN
2	k	159	GLN
2	k	203	GLN
2	k	226	ASN
2	k	331	GLN
2	l	113	GLN
2	l	159	GLN
2	l	203	GLN
2	l	226	ASN
2	l	331	GLN
2	m	113	GLN
2	m	159	GLN
2	m	203	GLN
2	m	226	ASN
2	m	331	GLN
2	n	113	GLN
2	n	159	GLN
2	n	203	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	n	226	ASN
2	n	331	GLN
2	o	113	GLN
2	o	159	GLN
2	o	203	GLN
2	o	226	ASN
2	o	331	GLN
2	p	113	GLN
2	p	159	GLN
2	p	203	GLN
2	p	226	ASN
2	p	331	GLN
2	q	113	GLN
2	q	159	GLN
2	q	203	GLN
2	q	226	ASN
2	q	331	GLN
2	r	113	GLN
2	r	159	GLN
2	r	203	GLN
2	r	226	ASN
2	r	331	GLN
2	s	113	GLN
2	s	159	GLN
2	s	203	GLN
2	s	226	ASN
2	s	331	GLN
2	t	113	GLN
2	t	159	GLN
2	t	203	GLN
2	t	226	ASN
2	t	331	GLN
2	u	113	GLN
2	u	159	GLN
2	u	203	GLN
2	u	226	ASN
2	u	331	GLN
2	v	113	GLN
2	v	159	GLN
2	v	203	GLN
2	v	226	ASN
2	v	331	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	w	113	GLN
2	w	159	GLN
2	w	203	GLN
2	w	226	ASN
2	w	331	GLN
2	x	113	GLN
2	x	159	GLN
2	x	203	GLN
2	x	226	ASN
2	x	331	GLN
2	y	113	GLN
2	y	159	GLN
2	y	203	GLN
2	y	226	ASN
2	y	331	GLN
2	z	113	GLN
2	z	159	GLN
2	z	203	GLN
2	z	226	ASN
2	z	331	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers [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-30398. 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](#)

This section was not generated.

### 6.2 Central slices [i](#)

This section was not generated.

### 6.3 Largest variance slices [i](#)

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views [i](#)

This section was not generated.

### 6.6 Mask visualisation [i](#)

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit

This section was not generated.