



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 05:48 PM JST

PDB ID : 7CBL  
EMDB ID : EMD-30335  
Title : Cryo-EM structure of the flagellar LP ring from Salmonella  
Authors : Tan, J.X.; Chang, S.H.; Wang, X.F.; Xu, C.H.; Zhou, Y.; Zhang, X.; Zhu, Y.Q.  
Deposited on : 2020-06-12  
Resolution : 2.80 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>.

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

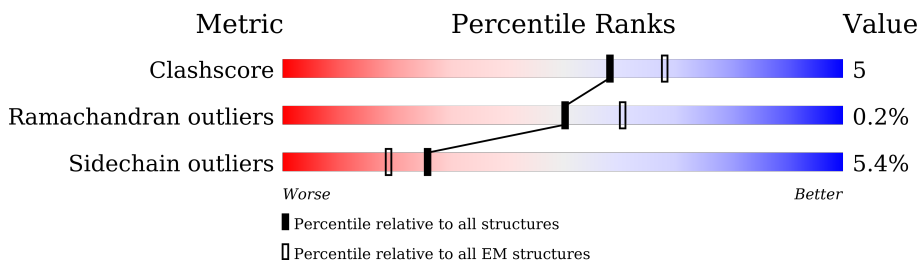
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 2.80 Å.

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









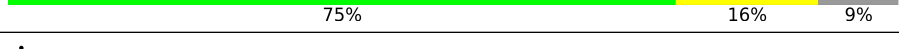
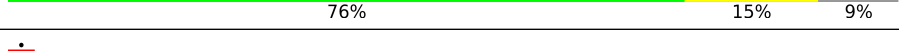
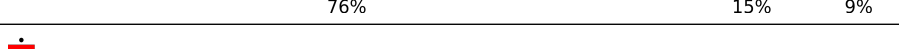
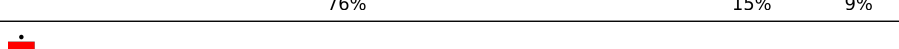
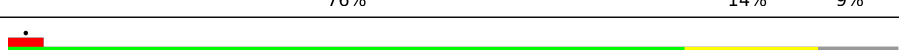

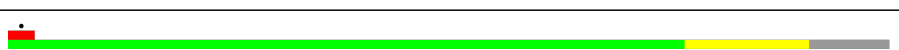

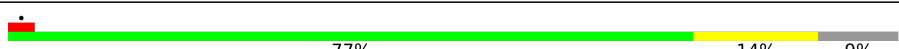





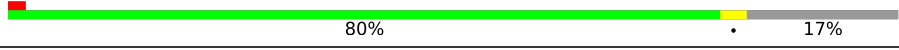
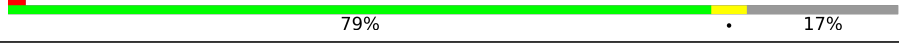



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	232	
1	B	232	
1	C	232	
1	D	232	
1	E	232	
1	F	232	
1	G	232	
1	H	232	






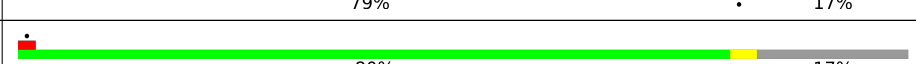
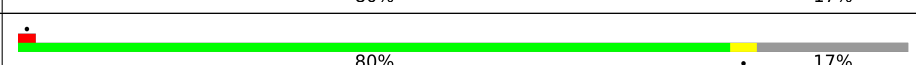
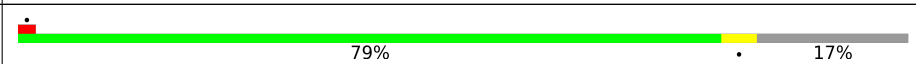


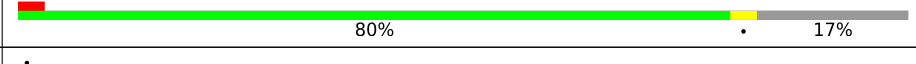
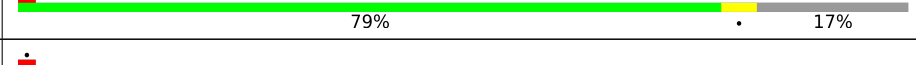
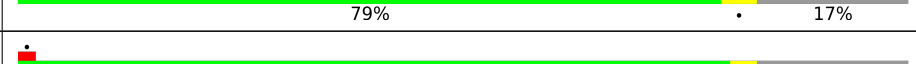
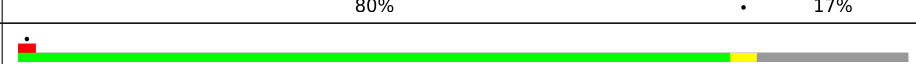
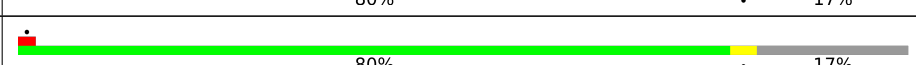




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Mol	Chain	Length	Quality of chain
1	I	232	 75% 15% 9%
1	J	232	 75% 16% 9%
1	K	232	 75% 15% 9%
1	L	232	 75% 15% 9%
1	M	232	 75% 16% 9%
1	N	232	 75% 16% 9%
1	O	232	 75% 16% 9%
1	P	232	 76% 15% 9%
1	Q	232	 76% 15% 9%
1	R	232	 76% 15% 9%
1	S	232	 76% 14% 9%
1	T	232	 76% 15% 9%
1	U	232	 76% 14% 9%
1	V	232	 76% 14% 9%
1	W	232	 75% 15% 9%
1	X	232	 77% 14% 9%
1	Y	232	 76% 14% 9%
1	Z	232	 76% 14% 9%
2	a	365	 79% . 17%
2	b	365	 80% . 17%
2	c	365	 79% . 17%
2	d	365	 80% . 17%
2	e	365	 79% . 17%
2	f	365	 80% . 17%
2	g	365	 79% . 17%

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Mol	Chain	Length	Quality of chain
2	h	365	 79% 17%
2	i	365	 80% 17%
2	j	365	 80% 17%
2	k	365	 79% 17%
2	l	365	 80% 17%
2	m	365	 79% 17%
2	n	365	 80% 17%
2	o	365	 80% 17%
2	p	365	 79% 17%
2	q	365	 80% 17%
2	r	365	 79% 17%
2	s	365	 80% 17%
2	t	365	 79% 17%
2	u	365	 79% 17%
2	v	365	 80% 17%
2	w	365	 80% 17%
2	x	365	 80% 17%
2	y	365	 79% 17%
2	z	365	 80% 17%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 99242 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
			Total	C	N	O	S		
1	A	211	1580	985	282	309	4	0	0
1	B	211	1580	985	282	309	4	0	0
1	C	211	1580	985	282	309	4	0	0
1	D	211	1580	985	282	309	4	0	0
1	E	211	1580	985	282	309	4	0	0
1	F	211	1580	985	282	309	4	0	0
1	G	211	1580	985	282	309	4	0	0
1	H	211	1580	985	282	309	4	0	0
1	I	211	1580	985	282	309	4	0	0
1	J	211	1580	985	282	309	4	0	0
1	K	211	1580	985	282	309	4	0	0
1	L	211	1580	985	282	309	4	0	0
1	M	211	1580	985	282	309	4	0	0
1	N	211	1580	985	282	309	4	0	0
1	O	211	1580	985	282	309	4	0	0
1	P	211	1580	985	282	309	4	0	0
1	Q	211	1580	985	282	309	4	0	0

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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.

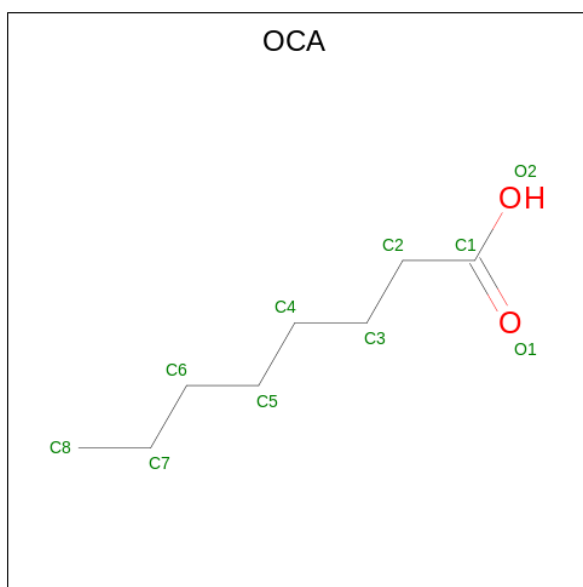
Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	b	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	c	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	d	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13		
2	e	303	Total	C	N	O	S	0	0
			2228	1364	405	446	13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

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

- Molecule 3 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula:  $C_8H_{16}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	8	1	
3	B	1	Total	C	O	0
			9	8	1	
3	C	1	Total	C	O	0
			9	8	1	
3	D	1	Total	C	O	0
			9	8	1	
3	E	1	Total	C	O	0
			9	8	1	
3	F	1	Total	C	O	0
			9	8	1	
3	G	1	Total	C	O	0
			9	8	1	
3	H	1	Total	C	O	0
			9	8	1	
3	I	1	Total	C	O	0
			9	8	1	
3	J	1	Total	C	O	0
			9	8	1	
3	K	1	Total	C	O	0
			9	8	1	
3	L	1	Total	C	O	0
			9	8	1	
3	M	1	Total	C	O	0
			9	8	1	
3	N	1	Total	C	O	0
			9	8	1	

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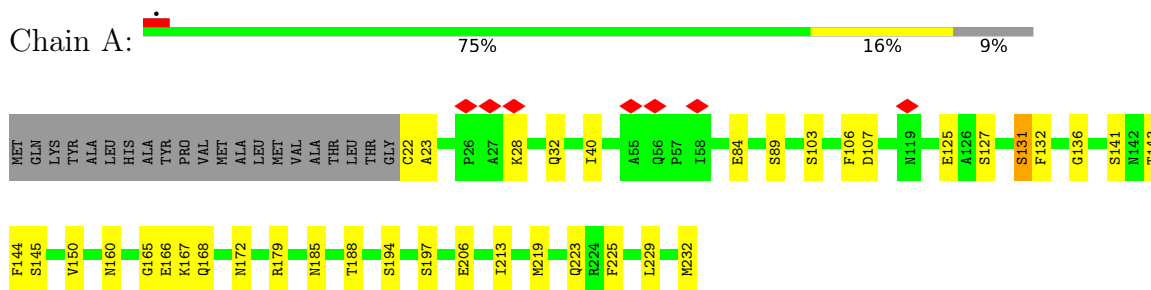
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Mol	Chain	Residues	Atoms			AltConf
3	O	1	Total	C	O	0
			9	8	1	
3	P	1	Total	C	O	0
			9	8	1	
3	Q	1	Total	C	O	0
			9	8	1	
3	R	1	Total	C	O	0
			9	8	1	
3	S	1	Total	C	O	0
			9	8	1	
3	T	1	Total	C	O	0
			9	8	1	
3	U	1	Total	C	O	0
			9	8	1	
3	V	1	Total	C	O	0
			9	8	1	
3	W	1	Total	C	O	0
			9	8	1	
3	X	1	Total	C	O	0
			9	8	1	
3	Y	1	Total	C	O	0
			9	8	1	
3	Z	1	Total	C	O	0
			9	8	1	

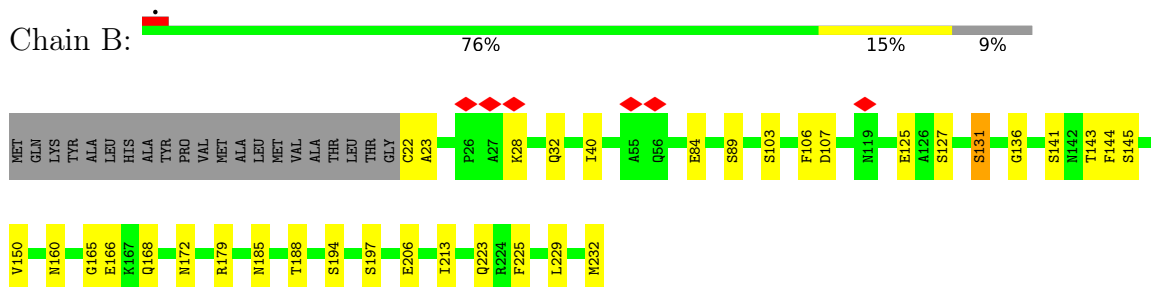
### 3 Residue-property plots

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

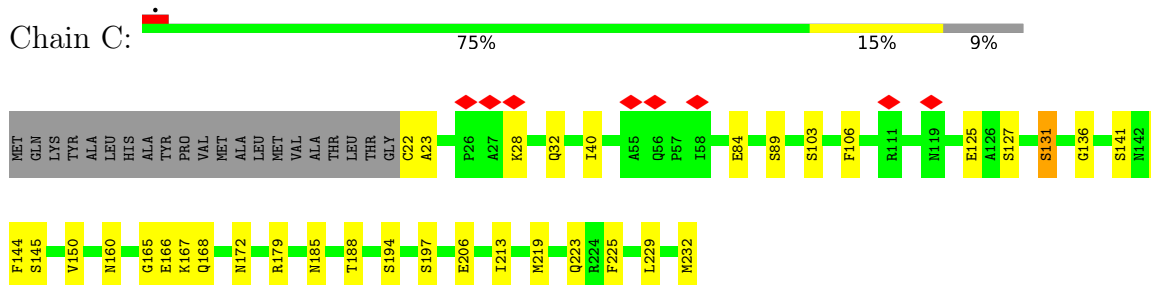
- Molecule 1: Flagellar L-ring protein



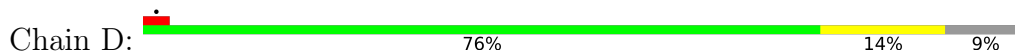
- Molecule 1: Flagellar L-ring protein

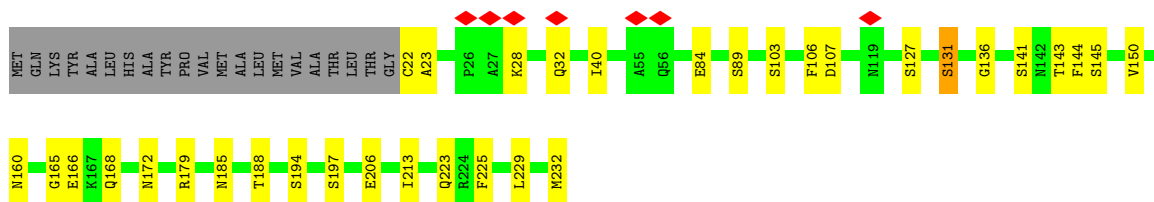


- Molecule 1: Flagellar L-ring protein

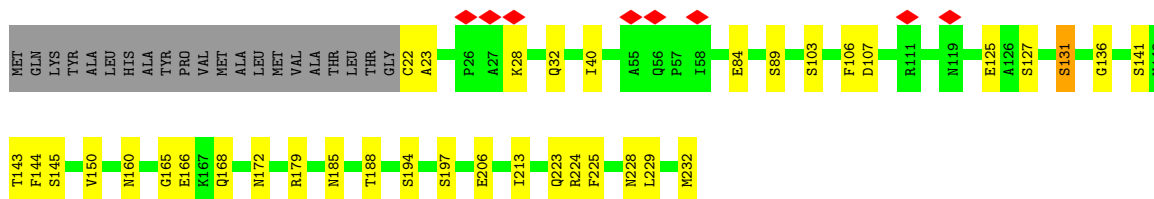
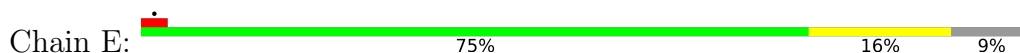


- Molecule 1: Flagellar L-ring protein

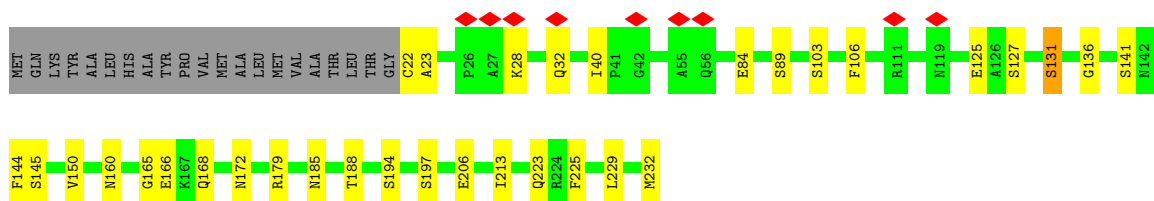
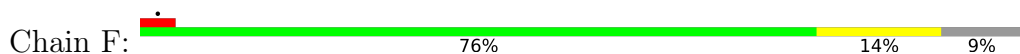




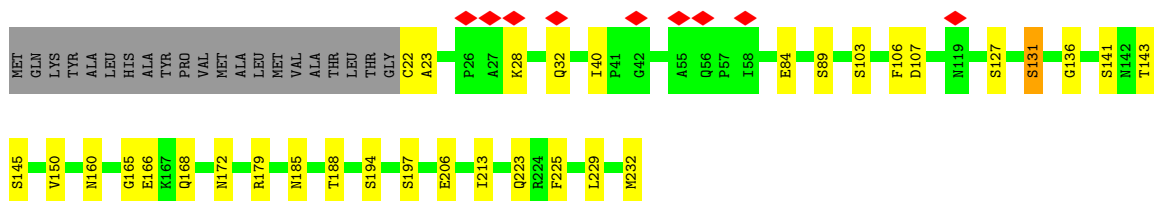
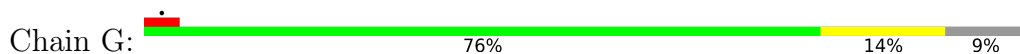
- Molecule 1: Flagellar L-ring protein



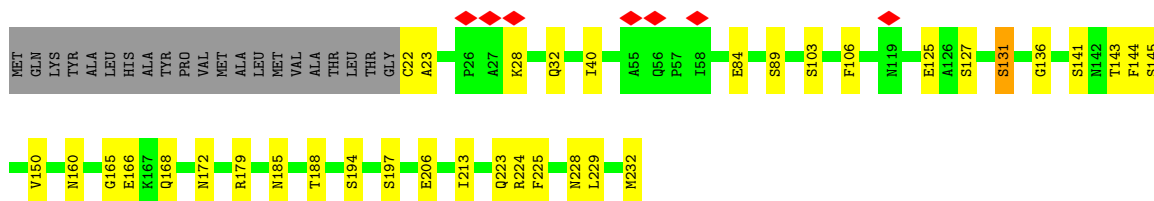
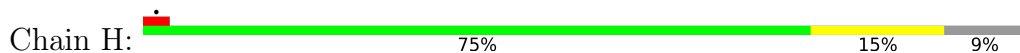
- Molecule 1: Flagellar L-ring protein



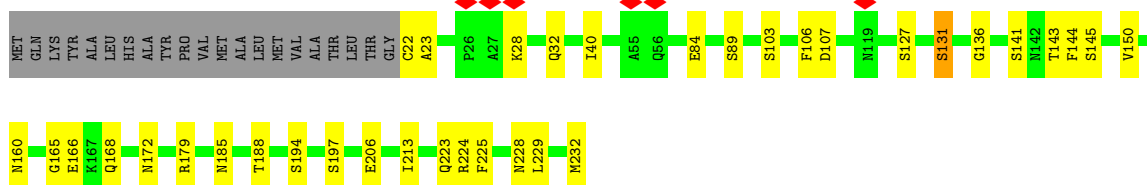
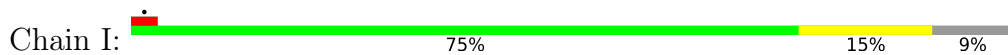
- Molecule 1: Flagellar L-ring protein



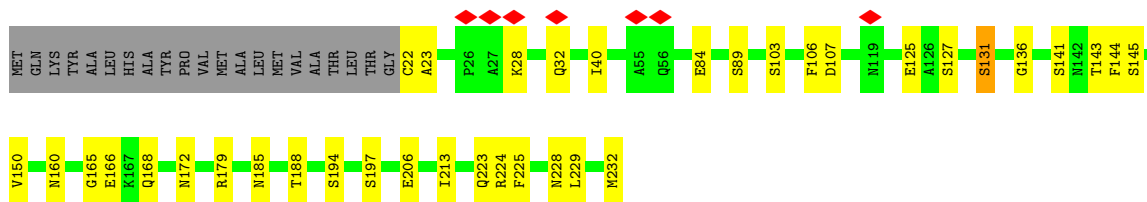
- Molecule 1: Flagellar L-ring protein



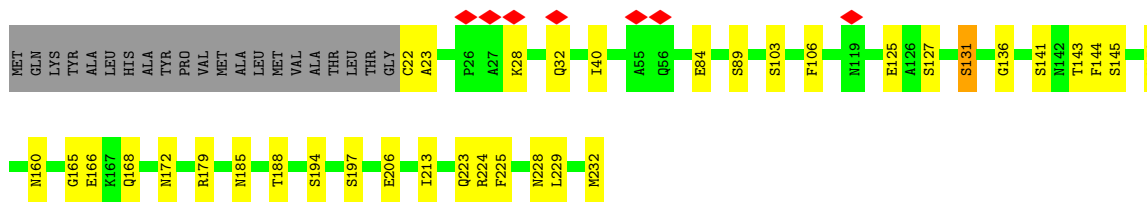
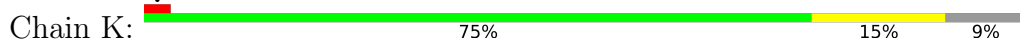
- Molecule 1: Flagellar L-ring protein



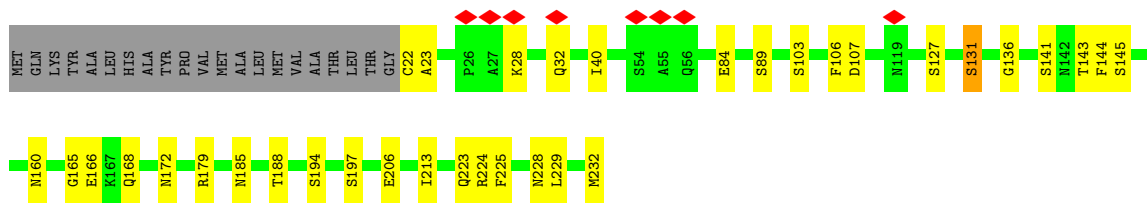
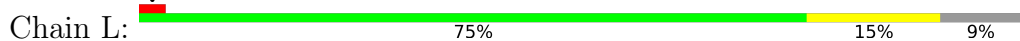
• Molecule 1: Flagellar L-ring protein



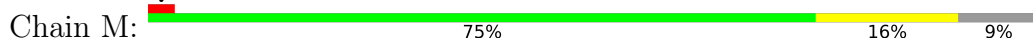
• Molecule 1: Flagellar L-ring protein



• Molecule 1: Flagellar L-ring protein

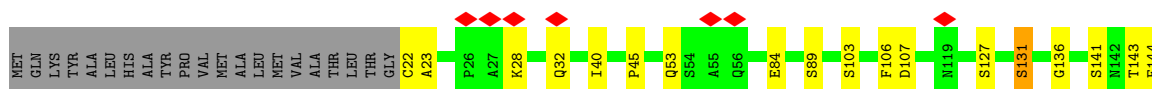
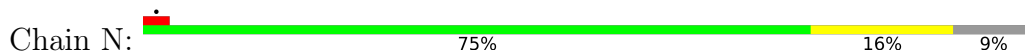


• Molecule 1: Flagellar L-ring protein

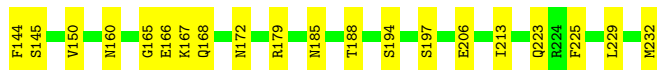
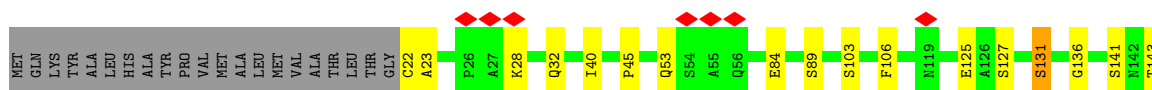
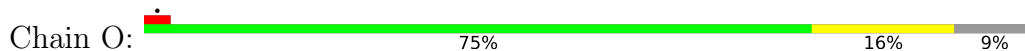




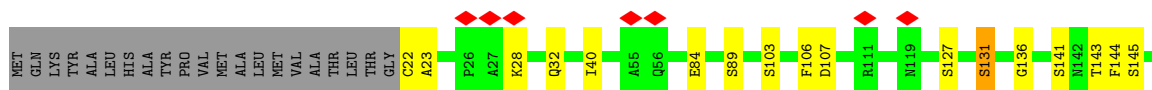
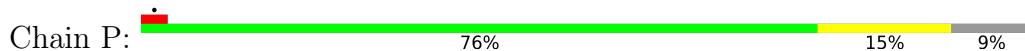
• Molecule 1: Flagellar L-ring protein



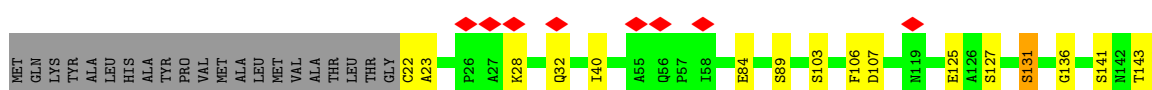
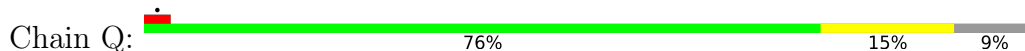
• Molecule 1: Flagellar L-ring protein



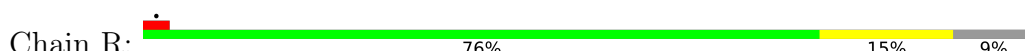
• Molecule 1: Flagellar L-ring protein

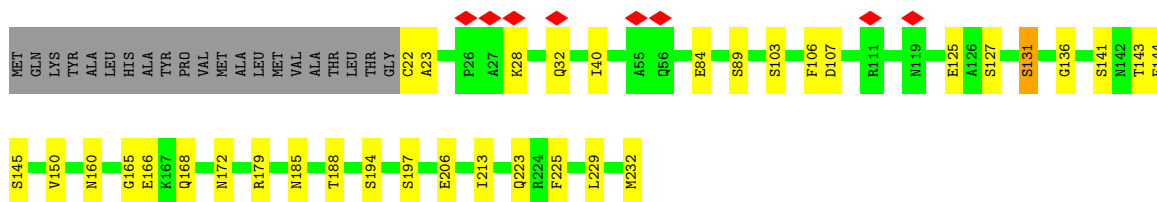


• Molecule 1: Flagellar L-ring protein

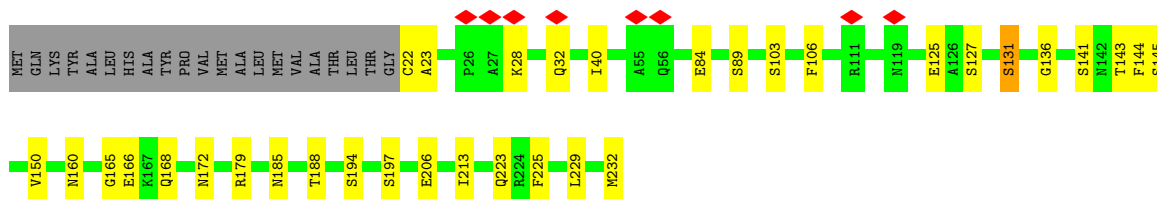
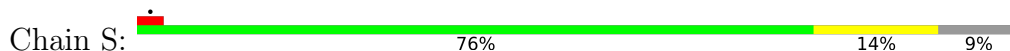


• Molecule 1: Flagellar L-ring protein

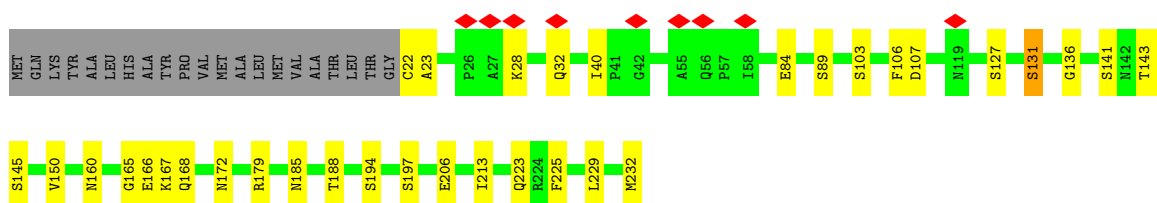
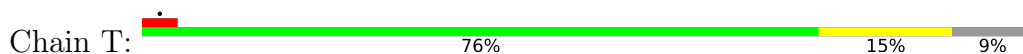




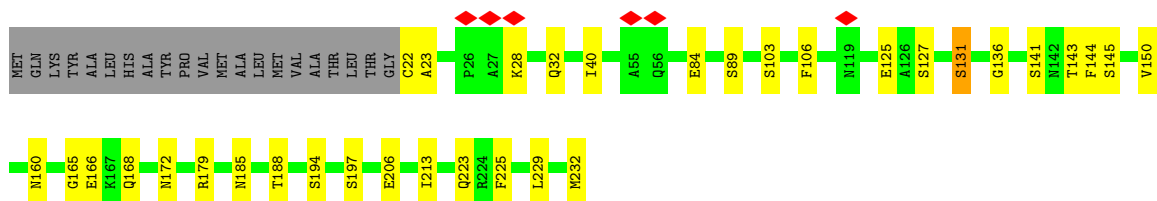
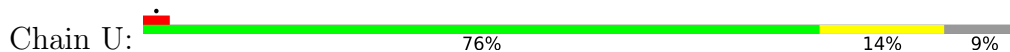
• Molecule 1: Flagellar L-ring protein



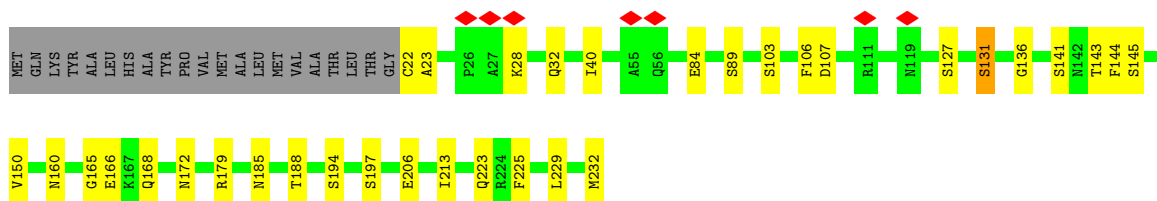
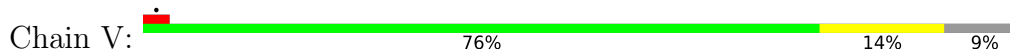
• Molecule 1: Flagellar L-ring protein



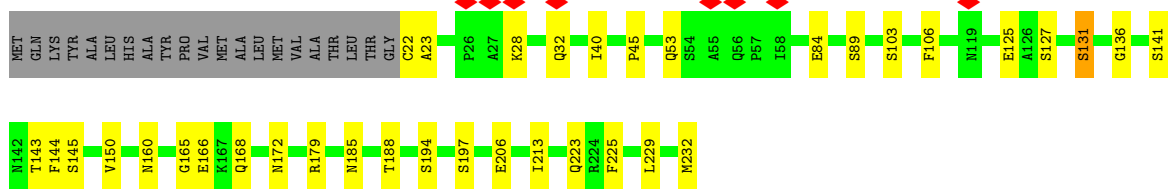
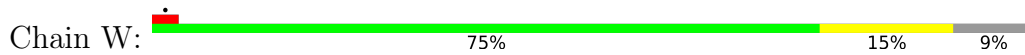
• Molecule 1: Flagellar L-ring protein



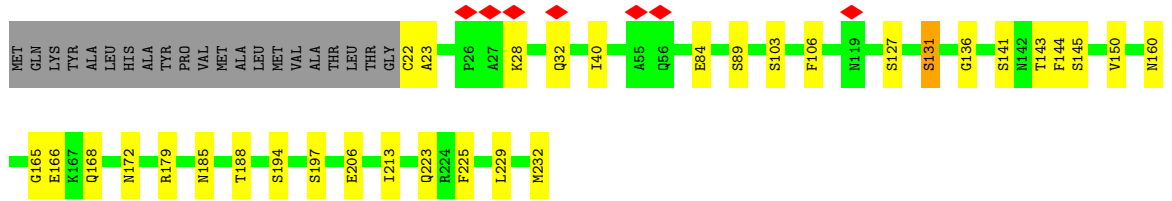
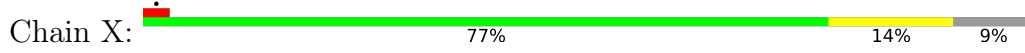
• Molecule 1: Flagellar L-ring protein



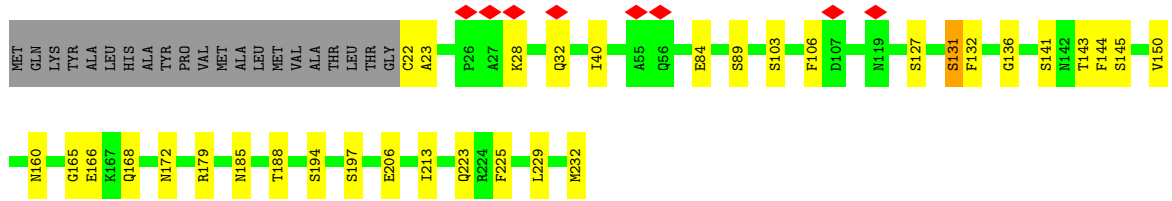
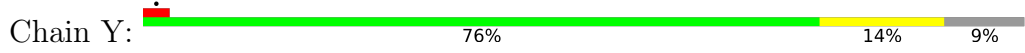
• Molecule 1: Flagellar L-ring protein



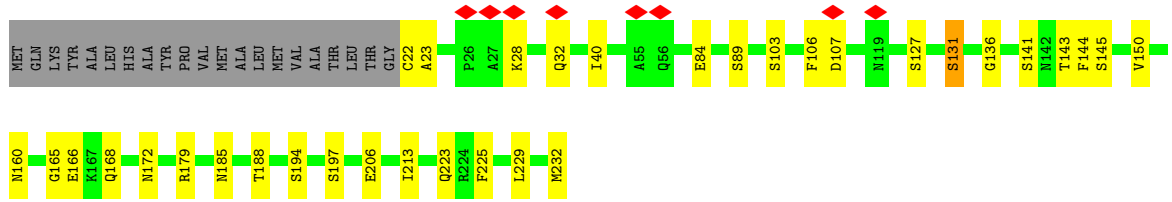
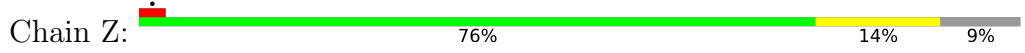
• Molecule 1: Flagellar L-ring protein



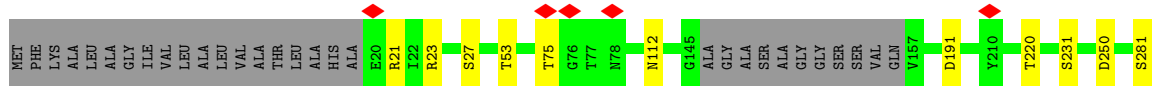
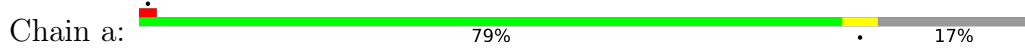
• Molecule 1: Flagellar L-ring protein

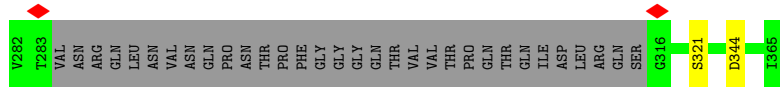


• Molecule 1: Flagellar L-ring protein

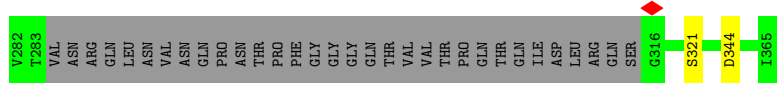
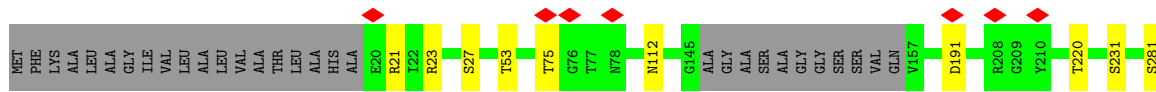
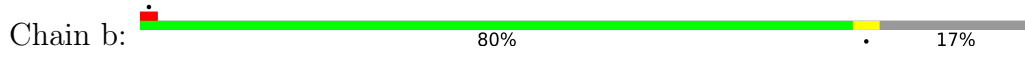


• Molecule 2: Flagellar P-ring protein

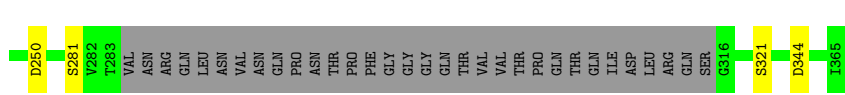
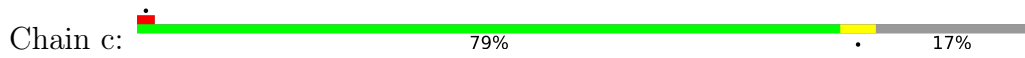




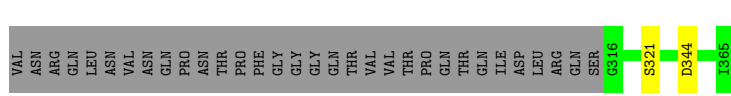
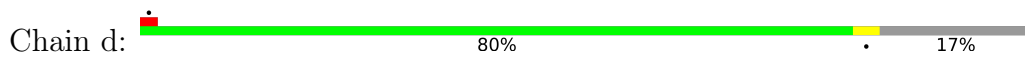
• Molecule 2: Flagellar P-ring protein



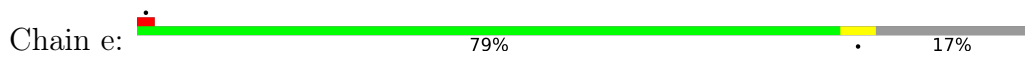
• Molecule 2: Flagellar P-ring protein



• Molecule 2: Flagellar P-ring protein

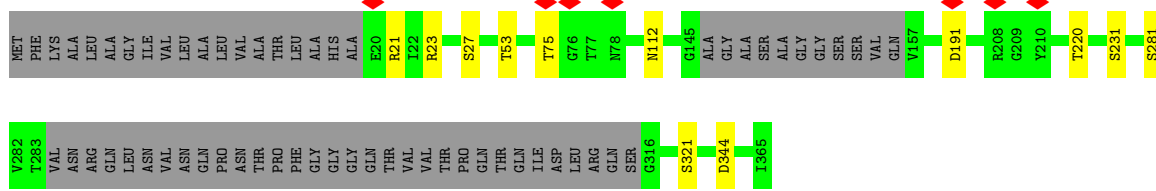
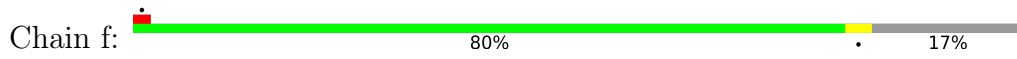


• Molecule 2: Flagellar P-ring protein

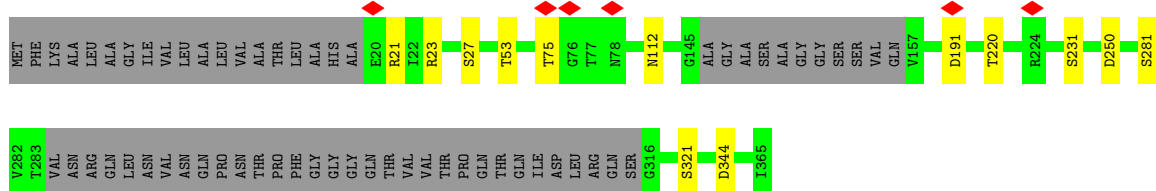
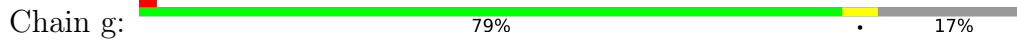


• Molecule 2: Flagellar P-ring protein

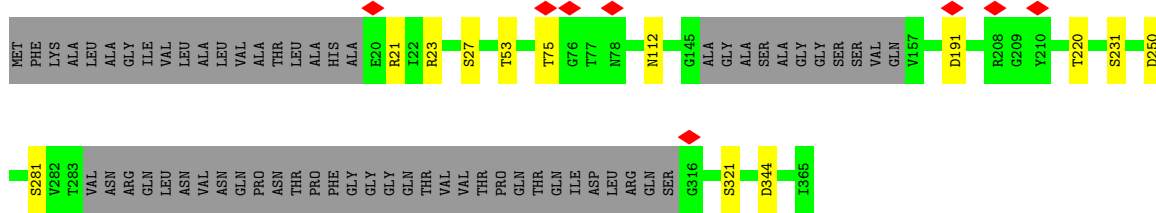
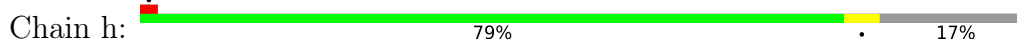




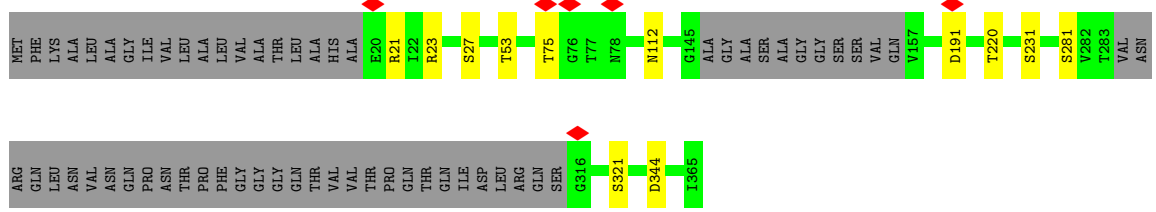
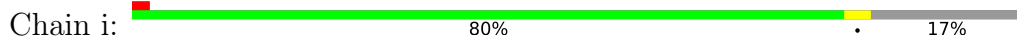
• Molecule 2: Flagellar P-ring protein



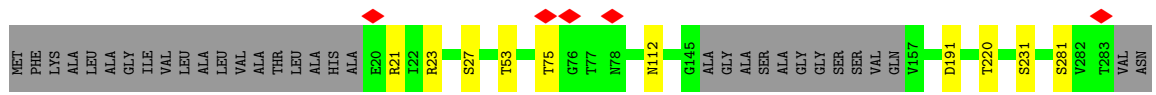
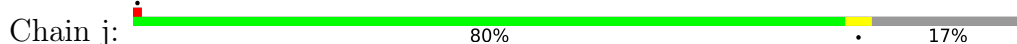
• Molecule 2: Flagellar P-ring protein

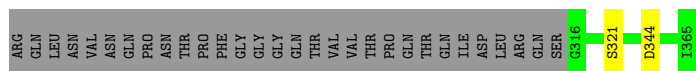


• Molecule 2: Flagellar P-ring protein

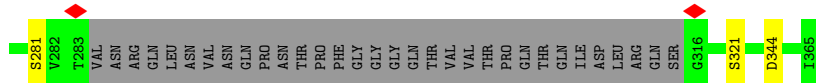
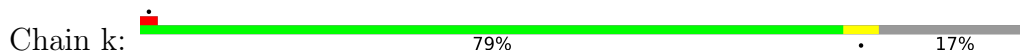


• Molecule 2: Flagellar P-ring protein

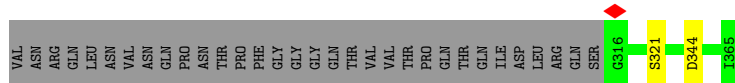
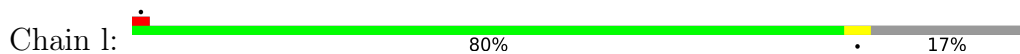




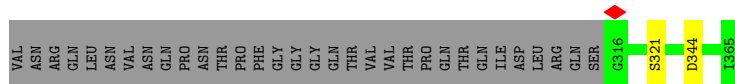
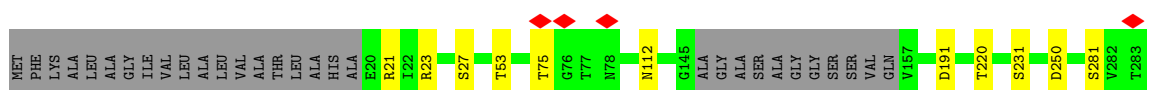
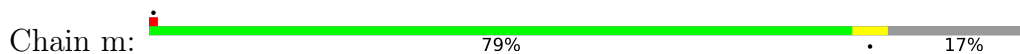
• Molecule 2: Flagellar P-ring protein



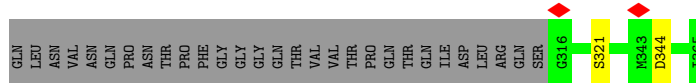
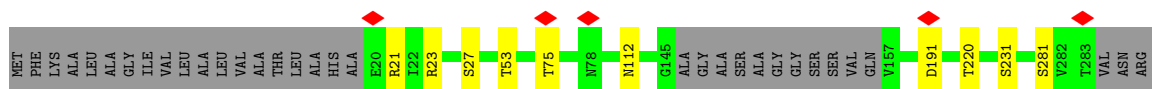
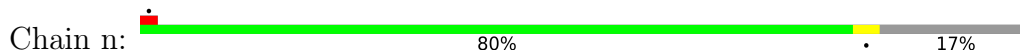
• Molecule 2: Flagellar P-ring protein



• Molecule 2: Flagellar P-ring protein

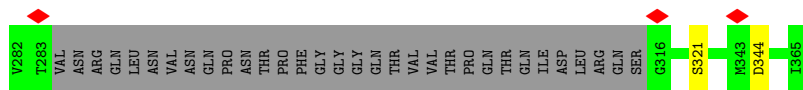


• Molecule 2: Flagellar P-ring protein

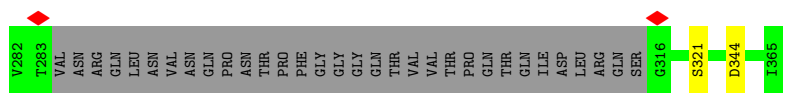
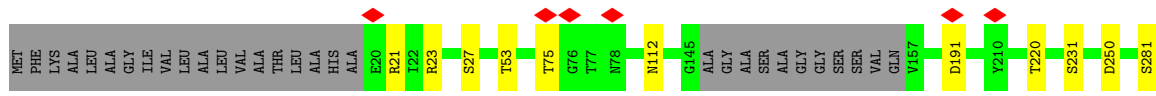
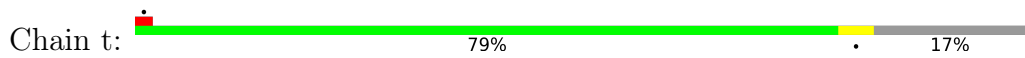


• Molecule 2: Flagellar P-ring protein

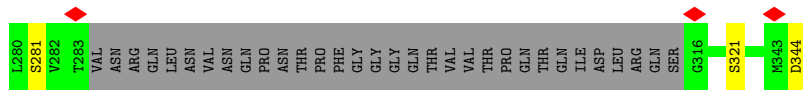
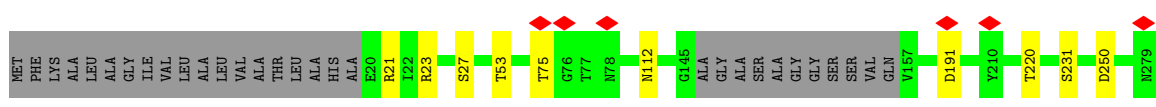
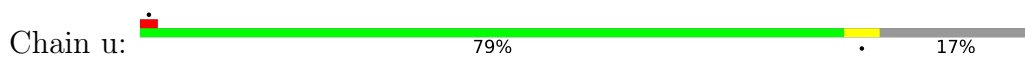




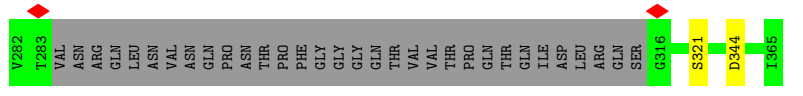
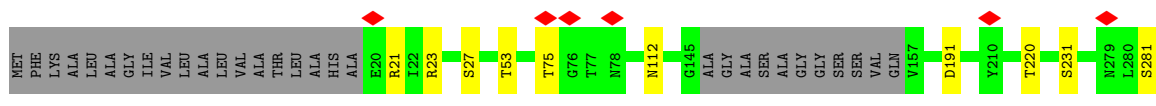
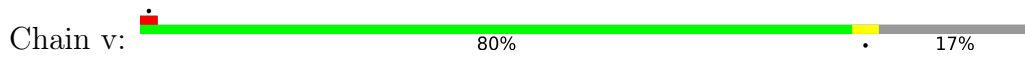
• Molecule 2: Flagellar P-ring protein



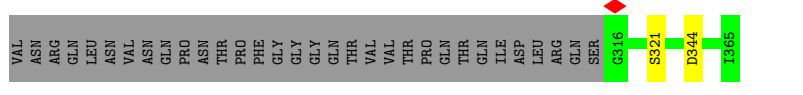
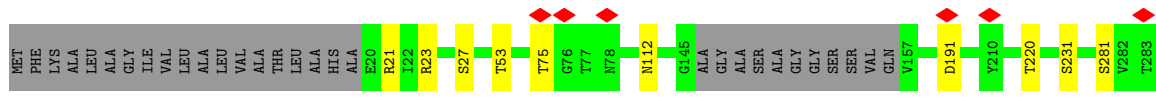
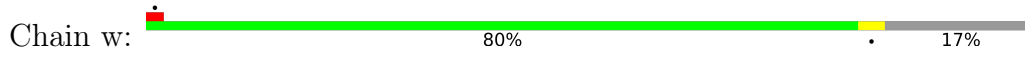
• Molecule 2: Flagellar P-ring protein



• Molecule 2: Flagellar P-ring protein

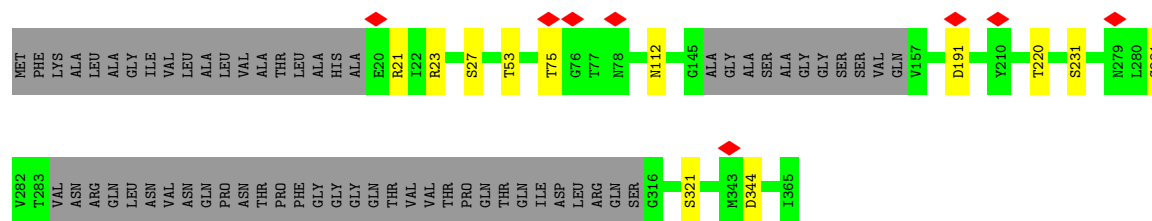


• Molecule 2: Flagellar P-ring protein



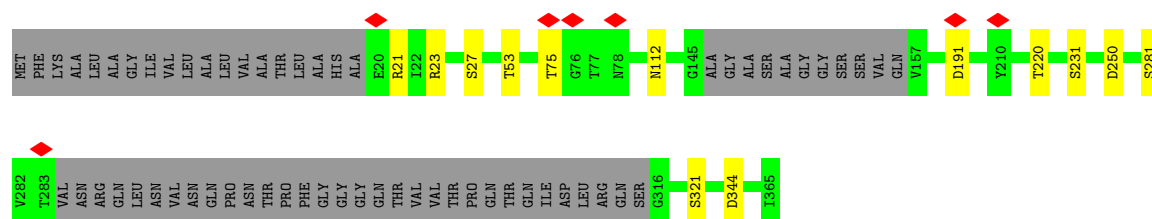
• Molecule 2: Flagellar P-ring protein

Chain x: 80% 17%



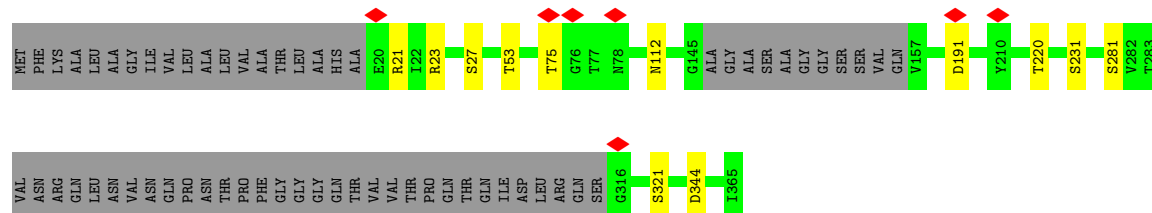
• Molecule 2: Flagellar P-ring protein

Chain y: 79% 17%



• Molecule 2: Flagellar P-ring protein

Chain z: 80% 17%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C26	Depositor
Number of particles used	80548	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 ( $e^-/\text{\AA}^2$ )	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.407	Depositor
Minimum map value	-3.040	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.809	Depositor
Map size (Å)	669.184, 669.184, 669.184	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
OCA

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	0.36	0/1613	0.48	0/2194
1	B	0.36	0/1613	0.48	0/2194
1	C	0.36	0/1613	0.48	0/2194
1	D	0.36	0/1613	0.48	0/2194
1	E	0.36	0/1613	0.48	0/2194
1	F	0.36	0/1613	0.48	0/2194
1	G	0.36	0/1613	0.48	0/2194
1	H	0.36	0/1613	0.48	0/2194
1	I	0.36	0/1613	0.48	0/2194
1	J	0.36	0/1613	0.48	0/2194
1	K	0.36	0/1613	0.48	0/2194
1	L	0.36	0/1613	0.48	0/2194
1	M	0.36	0/1613	0.48	0/2194
1	N	0.36	0/1613	0.48	0/2194
1	O	0.36	0/1613	0.48	0/2194
1	P	0.36	0/1613	0.48	0/2194
1	Q	0.36	0/1613	0.48	0/2194
1	R	0.36	0/1613	0.48	0/2194
1	S	0.36	0/1613	0.48	0/2194
1	T	0.36	0/1613	0.48	0/2194
1	U	0.36	0/1613	0.48	0/2194
1	V	0.36	0/1613	0.48	0/2194
1	W	0.36	0/1613	0.48	0/2194
1	X	0.36	0/1613	0.48	0/2194
1	Y	0.36	0/1613	0.48	0/2194
1	Z	0.36	0/1613	0.48	0/2194
2	a	0.33	0/2243	0.47	0/3041
2	b	0.33	0/2243	0.47	0/3041
2	c	0.33	0/2243	0.47	0/3041
2	d	0.33	0/2243	0.47	0/3041
2	e	0.33	0/2243	0.47	0/3041
2	f	0.33	0/2243	0.47	0/3041

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	g	0.33	0/2243	0.47	0/3041
2	h	0.33	0/2243	0.47	0/3041
2	i	0.33	0/2243	0.47	0/3041
2	j	0.33	0/2243	0.47	0/3041
2	k	0.33	0/2243	0.47	0/3041
2	l	0.33	0/2243	0.47	0/3041
2	m	0.33	0/2243	0.47	0/3041
2	n	0.33	0/2243	0.47	0/3041
2	o	0.33	0/2243	0.47	0/3041
2	p	0.33	0/2243	0.47	0/3041
2	q	0.33	0/2243	0.47	0/3041
2	r	0.33	0/2243	0.47	0/3041
2	s	0.33	0/2243	0.47	0/3041
2	t	0.33	0/2243	0.47	0/3041
2	u	0.33	0/2243	0.47	0/3041
2	v	0.33	0/2243	0.47	0/3041
2	w	0.33	0/2243	0.47	0/3041
2	x	0.33	0/2243	0.47	0/3041
2	y	0.33	0/2243	0.47	0/3041
2	z	0.33	0/2243	0.47	0/3041
All	All	0.34	0/100256	0.47	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	1533	22	0
1	B	1580	0	1533	20	0
1	C	1580	0	1533	19	0
1	D	1580	0	1533	17	0
1	E	1580	0	1533	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1580	0	1533	18	0
1	G	1580	0	1533	18	0
1	H	1580	0	1533	19	0
1	I	1580	0	1533	19	0
1	J	1580	0	1533	19	0
1	K	1580	0	1533	18	0
1	L	1580	0	1533	20	0
1	M	1580	0	1533	21	0
1	N	1580	0	1533	20	0
1	O	1580	0	1533	20	0
1	P	1580	0	1533	19	0
1	Q	1580	0	1533	19	0
1	R	1580	0	1533	19	0
1	S	1580	0	1533	18	0
1	T	1580	0	1533	19	0
1	U	1580	0	1533	18	0
1	V	1580	0	1533	18	0
1	W	1580	0	1533	19	0
1	X	1580	0	1533	17	0
1	Y	1580	0	1533	18	0
1	Z	1580	0	1533	19	0
2	a	2228	0	2265	0	0
2	b	2228	0	2265	0	0
2	c	2228	0	2265	0	0
2	d	2228	0	2265	0	0
2	e	2228	0	2265	0	0
2	f	2228	0	2265	0	0
2	g	2228	0	2265	0	0
2	h	2228	0	2265	0	0
2	i	2228	0	2265	0	0
2	j	2228	0	2265	0	0
2	k	2228	0	2265	0	0
2	l	2228	0	2265	0	0
2	m	2228	0	2265	0	0
2	n	2228	0	2265	0	0
2	o	2228	0	2265	0	0
2	p	2228	0	2265	0	0
2	q	2228	0	2265	0	0
2	r	2228	0	2265	0	0
2	s	2228	0	2265	0	0
2	t	2228	0	2265	0	0
2	u	2228	0	2265	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	v	2228	0	2265	0	0
2	w	2228	0	2265	0	0
2	x	2228	0	2265	0	0
2	y	2228	0	2265	0	0
2	z	2228	0	2265	0	0
3	A	9	0	15	1	0
3	B	9	0	15	1	0
3	C	9	0	15	0	0
3	D	9	0	15	0	0
3	E	9	0	15	1	0
3	F	9	0	15	1	0
3	G	9	0	15	1	0
3	H	9	0	15	1	0
3	I	9	0	15	1	0
3	J	9	0	15	0	0
3	K	9	0	15	0	0
3	L	9	0	15	1	0
3	M	9	0	15	1	0
3	N	9	0	15	0	0
3	O	9	0	15	0	0
3	P	9	0	15	1	0
3	Q	9	0	15	1	0
3	R	9	0	15	1	0
3	S	9	0	15	0	0
3	T	9	0	15	1	0
3	U	9	0	15	1	0
3	V	9	0	15	1	0
3	W	9	0	15	1	0
3	X	9	0	15	1	0
3	Y	9	0	15	1	0
3	Z	9	0	15	1	0
All	All	99242	0	99138	391	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 5.

All (391) 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:A:223:GLN:NE2	1:Y:131:SER:O	2.23	0.70
1:A:131:SER:O	1:C:223:GLN:NE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:131:SER:O	1:X:223:GLN:NE2	2.28	0.67
1:G:131:SER:O	1:I:223:GLN:NE2	2.28	0.67
1:M:131:SER:O	1:O:223:GLN:NE2	2.27	0.66
1:B:223:GLN:NE2	1:Z:131:SER:O	2.28	0.66
1:E:131:SER:O	1:G:223:GLN:NE2	2.28	0.66
1:C:131:SER:O	1:E:223:GLN:NE2	2.29	0.66
1:F:131:SER:O	1:H:223:GLN:NE2	2.29	0.66
1:L:131:SER:O	1:N:223:GLN:NE2	2.28	0.66
1:B:131:SER:O	1:D:223:GLN:NE2	2.29	0.66
1:H:131:SER:O	1:J:223:GLN:NE2	2.29	0.65
1:D:131:SER:O	1:F:223:GLN:NE2	2.29	0.65
1:P:22:CYS:SG	1:P:23:ALA:N	2.70	0.65
1:T:22:CYS:SG	1:T:23:ALA:N	2.70	0.65
1:W:22:CYS:SG	1:W:23:ALA:N	2.70	0.65
1:W:131:SER:O	1:Y:223:GLN:NE2	2.30	0.65
1:X:22:CYS:SG	1:X:23:ALA:N	2.70	0.65
1:Y:22:CYS:SG	1:Y:23:ALA:N	2.70	0.65
1:E:22:CYS:SG	1:E:23:ALA:N	2.70	0.65
1:F:22:CYS:SG	1:F:23:ALA:N	2.70	0.65
1:L:22:CYS:SG	1:L:23:ALA:N	2.70	0.65
1:M:22:CYS:SG	1:M:23:ALA:N	2.70	0.65
1:N:131:SER:O	1:P:223:GLN:NE2	2.29	0.65
1:Q:22:CYS:SG	1:Q:23:ALA:N	2.70	0.65
1:D:22:CYS:SG	1:D:23:ALA:N	2.70	0.64
1:U:22:CYS:SG	1:U:23:ALA:N	2.70	0.64
1:V:22:CYS:SG	1:V:23:ALA:N	2.70	0.64
1:N:22:CYS:SG	1:N:23:ALA:N	2.70	0.64
1:X:131:SER:O	1:Z:223:GLN:NE2	2.30	0.64
1:Z:22:CYS:SG	1:Z:23:ALA:N	2.70	0.64
1:G:22:CYS:SG	1:G:23:ALA:N	2.70	0.64
1:R:131:SER:O	1:T:223:GLN:NE2	2.29	0.64
1:K:131:SER:O	1:M:223:GLN:NE2	2.30	0.64
1:O:22:CYS:SG	1:O:23:ALA:N	2.70	0.64
1:H:22:CYS:SG	1:H:23:ALA:N	2.70	0.64
1:Q:131:SER:O	1:S:223:GLN:NE2	2.30	0.64
1:U:131:SER:O	1:W:223:GLN:NE2	2.31	0.64
1:B:22:CYS:SG	1:B:23:ALA:N	2.70	0.64
1:R:22:CYS:SG	1:R:23:ALA:N	2.70	0.64
1:S:22:CYS:SG	1:S:23:ALA:N	2.70	0.64
1:A:22:CYS:SG	1:A:23:ALA:N	2.70	0.64
1:O:131:SER:O	1:Q:223:GLN:NE2	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:CYS:SG	1:C:23:ALA:N	2.70	0.64
1:I:22:CYS:SG	1:I:23:ALA:N	2.70	0.63
1:J:22:CYS:SG	1:J:23:ALA:N	2.70	0.63
1:I:131:SER:O	1:K:223:GLN:NE2	2.30	0.63
1:J:131:SER:O	1:L:223:GLN:NE2	2.30	0.63
1:K:22:CYS:SG	1:K:23:ALA:N	2.70	0.63
1:P:131:SER:O	1:R:223:GLN:NE2	2.32	0.62
1:S:131:SER:O	1:U:223:GLN:NE2	2.30	0.62
1:L:232:MET:HG2	1:M:223:GLN:HB2	1.82	0.62
1:T:131:SER:O	1:V:223:GLN:NE2	2.32	0.62
1:B:232:MET:HG2	1:C:223:GLN:HB2	1.82	0.62
1:C:84:GLU:OE2	1:C:197:SER:OG	2.17	0.62
1:D:84:GLU:OE2	1:D:197:SER:OG	2.18	0.62
1:A:84:GLU:OE2	1:A:197:SER:OG	2.17	0.62
1:E:84:GLU:OE2	1:E:197:SER:OG	2.17	0.62
1:Q:232:MET:HG2	1:R:223:GLN:HB2	1.82	0.62
1:A:213:ILE:HG23	1:Y:136:GLY:HA3	1.80	0.62
1:F:84:GLU:OE2	1:F:197:SER:OG	2.17	0.62
1:P:84:GLU:OE2	1:P:197:SER:OG	2.17	0.61
1:G:84:GLU:OE2	1:G:197:SER:OG	2.17	0.61
1:Q:84:GLU:OE2	1:Q:197:SER:OG	2.17	0.61
1:Y:84:GLU:OE2	1:Y:197:SER:OG	2.17	0.61
1:A:223:GLN:HB2	1:Z:232:MET:HG2	1.81	0.61
1:T:179:ARG:NH1	1:T:206:GLU:OE1	2.34	0.61
1:X:179:ARG:NH1	1:X:206:GLU:OE1	2.34	0.61
1:S:232:MET:HG2	1:T:223:GLN:HB2	1.82	0.61
1:U:179:ARG:NH1	1:U:206:GLU:OE1	2.34	0.61
1:V:84:GLU:OE2	1:V:197:SER:OG	2.17	0.61
1:D:232:MET:HG2	1:E:223:GLN:HB2	1.82	0.61
1:Q:179:ARG:NH1	1:Q:206:GLU:OE1	2.34	0.61
1:H:84:GLU:OE2	1:H:197:SER:OG	2.17	0.61
1:W:179:ARG:NH1	1:W:206:GLU:OE1	2.34	0.61
1:P:179:ARG:NH1	1:P:206:GLU:OE1	2.34	0.60
1:U:84:GLU:OE2	1:U:197:SER:OG	2.17	0.60
1:A:179:ARG:NH1	1:A:206:GLU:OE1	2.34	0.60
1:R:179:ARG:NH1	1:R:206:GLU:OE1	2.34	0.60
1:Y:179:ARG:NH1	1:Y:206:GLU:OE1	2.34	0.60
1:W:84:GLU:OE2	1:W:197:SER:OG	2.17	0.60
1:B:179:ARG:NH1	1:B:206:GLU:OE1	2.34	0.60
1:I:84:GLU:OE2	1:I:197:SER:OG	2.17	0.60
1:S:179:ARG:NH1	1:S:206:GLU:OE1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LYS:NZ	1:Z:84:GLU:OE1	2.25	0.60
1:N:179:ARG:NH1	1:N:206:GLU:OE1	2.34	0.60
1:M:179:ARG:NH1	1:M:206:GLU:OE1	2.34	0.60
1:V:179:ARG:NH1	1:V:206:GLU:OE1	2.34	0.60
1:Z:84:GLU:OE2	1:Z:197:SER:OG	2.18	0.60
1:Z:179:ARG:NH1	1:Z:206:GLU:OE1	2.34	0.60
1:J:84:GLU:OE2	1:J:197:SER:OG	2.17	0.60
1:J:232:MET:HG2	1:K:223:GLN:HB2	1.83	0.59
1:N:232:MET:HG2	1:O:223:GLN:HB2	1.84	0.59
1:E:179:ARG:NH1	1:E:206:GLU:OE1	2.34	0.59
1:X:84:GLU:OE2	1:X:197:SER:OG	2.17	0.59
1:U:232:MET:HG2	1:V:223:GLN:HB2	1.84	0.59
1:C:179:ARG:NH1	1:C:206:GLU:OE1	2.34	0.59
1:G:232:MET:HG2	1:H:223:GLN:HB2	1.85	0.59
1:I:179:ARG:NH1	1:I:206:GLU:OE1	2.34	0.59
1:L:179:ARG:NH1	1:L:206:GLU:OE1	2.34	0.59
1:O:179:ARG:NH1	1:O:206:GLU:OE1	2.34	0.59
1:R:84:GLU:OE2	1:R:197:SER:OG	2.17	0.59
1:V:232:MET:HG2	1:W:223:GLN:HB2	1.83	0.59
1:D:179:ARG:NH1	1:D:206:GLU:OE1	2.34	0.59
1:F:179:ARG:NH1	1:F:206:GLU:OE1	2.34	0.59
1:J:179:ARG:NH1	1:J:206:GLU:OE1	2.34	0.59
1:K:84:GLU:OE2	1:K:197:SER:OG	2.17	0.59
1:F:232:MET:HG2	1:G:223:GLN:HB2	1.85	0.59
1:B:84:GLU:OE2	1:B:197:SER:OG	2.18	0.59
1:Y:232:MET:HG2	1:Z:223:GLN:HB2	1.84	0.59
1:O:232:MET:HG2	1:P:223:GLN:HB2	1.84	0.59
1:I:232:MET:HG2	1:J:223:GLN:HB2	1.84	0.58
1:R:232:MET:HG2	1:S:223:GLN:HB2	1.85	0.58
1:H:179:ARG:NH1	1:H:206:GLU:OE1	2.34	0.58
1:E:232:MET:HG2	1:F:223:GLN:HB2	1.85	0.58
1:H:232:MET:HG2	1:I:223:GLN:HB2	1.86	0.58
1:L:84:GLU:OE2	1:L:197:SER:OG	2.17	0.58
1:K:179:ARG:NH1	1:K:206:GLU:OE1	2.34	0.58
1:S:84:GLU:OE2	1:S:197:SER:OG	2.18	0.58
1:T:232:MET:HG2	1:U:223:GLN:HB2	1.85	0.58
1:X:232:MET:HG2	1:Y:223:GLN:HB2	1.84	0.58
1:G:179:ARG:NH1	1:G:206:GLU:OE1	2.34	0.58
1:A:232:MET:HG2	1:B:223:GLN:HB2	1.85	0.58
1:P:232:MET:HG2	1:Q:223:GLN:HB2	1.85	0.58
1:M:84:GLU:OE2	1:M:197:SER:OG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:GLU:OE2	1:N:197:SER:OG	2.17	0.57
1:T:84:GLU:OE2	1:T:197:SER:OG	2.17	0.57
1:M:232:MET:HG2	1:N:223:GLN:HB2	1.87	0.57
1:K:232:MET:HG2	1:L:223:GLN:HB2	1.87	0.56
1:O:84:GLU:OE2	1:O:197:SER:OG	2.18	0.56
1:W:232:MET:HG2	1:X:223:GLN:HB2	1.86	0.56
1:C:232:MET:HG2	1:D:223:GLN:HB2	1.88	0.55
1:S:136:GLY:HA3	1:U:213:ILE:HG23	1.92	0.51
1:N:136:GLY:HA3	1:P:213:ILE:HG23	1.93	0.51
1:R:136:GLY:HA3	1:T:213:ILE:HG23	1.93	0.51
1:O:136:GLY:HA3	1:Q:213:ILE:HG23	1.93	0.51
1:M:84:GLU:OE1	1:N:167:LYS:NZ	2.36	0.51
1:L:136:GLY:HA3	1:N:213:ILE:HG23	1.93	0.50
1:M:136:GLY:HA3	1:O:213:ILE:HG23	1.94	0.50
1:T:136:GLY:HA3	1:V:213:ILE:HG23	1.93	0.50
1:G:136:GLY:HA3	1:I:213:ILE:HG23	1.92	0.49
1:B:136:GLY:HA3	1:D:213:ILE:HG23	1.93	0.49
1:U:136:GLY:HA3	1:W:213:ILE:HG23	1.93	0.49
1:V:136:GLY:HA3	1:X:213:ILE:HG23	1.93	0.49
1:H:136:GLY:HA3	1:J:213:ILE:HG23	1.93	0.49
1:E:136:GLY:HA3	1:G:213:ILE:HG23	1.94	0.49
1:F:136:GLY:HA3	1:H:213:ILE:HG23	1.93	0.49
1:B:213:ILE:HG23	1:Z:136:GLY:HA3	1.94	0.48
1:P:136:GLY:HA3	1:R:213:ILE:HG23	1.95	0.48
1:Q:136:GLY:HA3	1:S:213:ILE:HG23	1.95	0.48
1:B:84:GLU:OE1	1:C:167:LYS:NZ	2.35	0.48
1:D:136:GLY:HA3	1:F:213:ILE:HG23	1.95	0.48
1:S:84:GLU:OE1	1:T:167:LYS:NZ	2.33	0.48
1:X:136:GLY:HA3	1:Z:213:ILE:HG23	1.94	0.48
1:H:22:CYS:HB2	3:H:301:OCA:H21	1.63	0.47
1:P:166:GLU:OE1	1:P:168:GLN:NE2	2.32	0.47
1:C:136:GLY:HA3	1:E:213:ILE:HG23	1.95	0.47
1:I:136:GLY:HA3	1:K:213:ILE:HG23	1.95	0.47
1:M:22:CYS:HB2	3:M:301:OCA:H21	1.63	0.47
1:A:136:GLY:HA3	1:C:213:ILE:HG23	1.96	0.47
1:L:84:GLU:OE1	1:M:167:LYS:NZ	2.35	0.47
1:W:166:GLU:OE1	1:W:168:GLN:NE2	2.32	0.47
1:X:166:GLU:OE1	1:X:168:GLN:NE2	2.32	0.47
1:Y:166:GLU:OE1	1:Y:168:GLN:NE2	2.32	0.47
1:Y:185:ASN:O	1:Y:188:THR:OG1	2.33	0.47
1:A:22:CYS:HB2	3:A:301:OCA:H21	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:O	1:B:188:THR:OG1	2.33	0.47
1:K:136:GLY:HA3	1:M:213:ILE:HG23	1.97	0.47
1:P:185:ASN:O	1:P:188:THR:OG1	2.33	0.47
1:G:185:ASN:O	1:G:188:THR:OG1	2.33	0.47
1:X:185:ASN:O	1:X:188:THR:OG1	2.33	0.47
1:Z:166:GLU:OE1	1:Z:168:GLN:NE2	2.32	0.47
1:V:166:GLU:OE1	1:V:168:GLN:NE2	2.32	0.47
1:H:225:PHE:CE1	1:H:229:LEU:HD12	2.51	0.46
1:I:225:PHE:CE1	1:I:229:LEU:HD12	2.51	0.46
1:J:225:PHE:CE1	1:J:229:LEU:HD12	2.51	0.46
1:O:166:GLU:OE1	1:O:168:GLN:NE2	2.32	0.46
1:X:225:PHE:CE1	1:X:229:LEU:HD12	2.51	0.46
1:G:225:PHE:CE1	1:G:229:LEU:HD12	2.51	0.46
1:K:225:PHE:CE1	1:K:229:LEU:HD12	2.51	0.46
1:L:225:PHE:CE1	1:L:229:LEU:HD12	2.51	0.46
1:N:84:GLU:OE1	1:O:167:LYS:NZ	2.36	0.46
1:Q:225:PHE:CE1	1:Q:229:LEU:HD12	2.51	0.46
1:F:225:PHE:CE1	1:F:229:LEU:HD12	2.51	0.46
1:T:185:ASN:O	1:T:188:THR:OG1	2.33	0.46
1:V:225:PHE:CE1	1:V:229:LEU:HD12	2.51	0.46
1:Z:225:PHE:CE1	1:Z:229:LEU:HD12	2.51	0.46
1:J:136:GLY:HA3	1:L:213:ILE:HG23	1.97	0.46
1:M:225:PHE:CE1	1:M:229:LEU:HD12	2.51	0.46
1:O:185:ASN:O	1:O:188:THR:OG1	2.33	0.46
1:S:225:PHE:CE1	1:S:229:LEU:HD12	2.50	0.46
1:T:225:PHE:CE1	1:T:229:LEU:HD12	2.51	0.46
1:E:225:PHE:CE1	1:E:229:LEU:HD12	2.51	0.46
1:R:225:PHE:CE1	1:R:229:LEU:HD12	2.51	0.46
1:A:166:GLU:OE1	1:A:168:GLN:NE2	2.32	0.46
1:A:225:PHE:CE1	1:A:229:LEU:HD12	2.51	0.46
1:F:185:ASN:O	1:F:188:THR:OG1	2.33	0.46
1:N:225:PHE:CE1	1:N:229:LEU:HD12	2.51	0.46
1:O:225:PHE:CE1	1:O:229:LEU:HD12	2.51	0.46
1:S:185:ASN:O	1:S:188:THR:OG1	2.33	0.46
1:U:166:GLU:OE1	1:U:168:GLN:NE2	2.32	0.46
1:W:185:ASN:O	1:W:188:THR:OG1	2.33	0.46
1:B:225:PHE:CE1	1:B:229:LEU:HD12	2.51	0.46
1:C:225:PHE:CE1	1:C:229:LEU:HD12	2.51	0.46
1:D:225:PHE:CE1	1:D:229:LEU:HD12	2.51	0.46
1:W:225:PHE:CE1	1:W:229:LEU:HD12	2.51	0.46
1:A:185:ASN:O	1:A:188:THR:OG1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:225:PHE:CE1	1:U:229:LEU:HD12	2.51	0.46
1:Y:225:PHE:CE1	1:Y:229:LEU:HD12	2.51	0.46
1:N:166:GLU:OE1	1:N:168:GLN:NE2	2.32	0.45
1:P:225:PHE:CE1	1:P:229:LEU:HD12	2.51	0.45
1:R:22:CYS:HB2	3:R:301:OCA:H21	1.63	0.45
1:W:136:GLY:HA3	1:Y:213:ILE:HG23	1.96	0.45
1:B:166:GLU:OE1	1:B:168:GLN:NE2	2.32	0.45
1:C:166:GLU:OE1	1:C:168:GLN:NE2	2.32	0.45
1:L:185:ASN:O	1:L:188:THR:OG1	2.33	0.45
1:M:185:ASN:O	1:M:188:THR:OG1	2.33	0.45
1:T:22:CYS:HB2	3:T:301:OCA:H21	1.63	0.45
1:B:22:CYS:HB2	3:B:301:OCA:H21	1.63	0.45
1:D:150:VAL:HG12	1:D:165:GLY:HA3	1.99	0.45
1:E:150:VAL:HG12	1:E:165:GLY:HA3	1.99	0.45
1:T:166:GLU:OE1	1:T:168:GLN:NE2	2.32	0.45
1:E:185:ASN:O	1:E:188:THR:OG1	2.33	0.45
1:F:150:VAL:HG12	1:F:165:GLY:HA3	1.99	0.45
1:G:150:VAL:HG12	1:G:165:GLY:HA3	1.99	0.45
1:N:185:ASN:O	1:N:188:THR:OG1	2.33	0.45
1:C:150:VAL:HG12	1:C:165:GLY:HA3	1.99	0.45
1:H:150:VAL:HG12	1:H:165:GLY:HA3	1.99	0.45
1:K:185:ASN:O	1:K:188:THR:OG1	2.33	0.45
1:R:185:ASN:O	1:R:188:THR:OG1	2.33	0.45
1:B:150:VAL:HG12	1:B:165:GLY:HA3	1.99	0.45
1:V:185:ASN:O	1:V:188:THR:OG1	2.33	0.45
1:Z:150:VAL:HG12	1:Z:165:GLY:HA3	1.99	0.45
1:A:150:VAL:HG12	1:A:165:GLY:HA3	1.99	0.44
1:I:150:VAL:HG12	1:I:165:GLY:HA3	1.99	0.44
1:M:166:GLU:OE1	1:M:168:GLN:NE2	2.32	0.44
1:Y:150:VAL:HG12	1:Y:165:GLY:HA3	1.99	0.44
1:J:150:VAL:HG12	1:J:165:GLY:HA3	1.99	0.44
1:O:84:GLU:OE1	1:P:167:LYS:NZ	2.36	0.44
1:Z:22:CYS:HB2	3:Z:301:OCA:H21	1.63	0.44
1:A:219:MET:HG2	1:Y:132:PHE:CD1	2.52	0.44
1:E:28:LYS:HE2	1:E:32:GLN:HE22	1.83	0.44
1:O:28:LYS:HE2	1:O:32:GLN:HE22	1.83	0.44
1:Z:28:LYS:HE2	1:Z:32:GLN:HE22	1.83	0.44
1:A:172:ASN:O	1:A:172:ASN:ND2	2.51	0.44
1:J:28:LYS:HE2	1:J:32:GLN:HE22	1.83	0.44
1:X:150:VAL:HG12	1:X:165:GLY:HA3	1.99	0.44
1:X:172:ASN:ND2	1:X:172:ASN:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:185:ASN:O	1:Z:188:THR:OG1	2.33	0.44
1:B:107:ASP:HB3	1:C:125:GLU:HG2	2.00	0.44
1:C:172:ASN:O	1:C:172:ASN:ND2	2.51	0.44
1:D:28:LYS:HE2	1:D:32:GLN:HE22	1.83	0.44
1:E:172:ASN:O	1:E:172:ASN:ND2	2.51	0.44
1:K:150:VAL:HG12	1:K:165:GLY:HA3	1.99	0.44
1:N:28:LYS:HE2	1:N:32:GLN:HE22	1.83	0.44
1:R:28:LYS:HE2	1:R:32:GLN:HE22	1.83	0.44
1:S:28:LYS:HE2	1:S:32:GLN:HE22	1.83	0.44
1:U:172:ASN:ND2	1:U:172:ASN:O	2.51	0.44
1:V:28:LYS:HE2	1:V:32:GLN:HE22	1.83	0.44
1:W:150:VAL:HG12	1:W:165:GLY:HA3	1.99	0.44
1:Y:28:LYS:HE2	1:Y:32:GLN:HE22	1.83	0.44
1:Z:172:ASN:ND2	1:Z:172:ASN:O	2.51	0.44
1:B:172:ASN:ND2	1:B:172:ASN:O	2.51	0.44
1:D:166:GLU:OE1	1:D:168:GLN:NE2	2.32	0.44
1:G:22:CYS:HB2	3:G:301:OCA:H21	1.63	0.44
1:J:185:ASN:O	1:J:188:THR:OG1	2.33	0.44
1:K:28:LYS:HE2	1:K:32:GLN:HE22	1.83	0.44
1:L:150:VAL:HG12	1:L:165:GLY:HA3	1.99	0.44
1:U:22:CYS:HB2	3:U:301:OCA:H21	1.63	0.44
1:A:28:LYS:HE2	1:A:32:GLN:HE22	1.83	0.44
1:D:172:ASN:ND2	1:D:172:ASN:O	2.51	0.44
1:I:28:LYS:HE2	1:I:32:GLN:HE22	1.83	0.44
1:M:150:VAL:HG12	1:M:165:GLY:HA3	1.99	0.44
1:P:150:VAL:HG12	1:P:165:GLY:HA3	1.99	0.44
1:Q:150:VAL:HG12	1:Q:165:GLY:HA3	1.99	0.44
1:Q:185:ASN:O	1:Q:188:THR:OG1	2.33	0.44
1:S:166:GLU:OE1	1:S:168:GLN:NE2	2.32	0.44
1:V:172:ASN:ND2	1:V:172:ASN:O	2.51	0.44
1:N:160:ASN:HD22	1:N:185:ASN:HA	1.83	0.44
1:O:160:ASN:HD22	1:O:185:ASN:HA	1.83	0.44
1:P:22:CYS:HB2	3:P:301:OCA:H21	1.63	0.44
1:P:160:ASN:HD22	1:P:185:ASN:HA	1.83	0.44
1:F:28:LYS:HE2	1:F:32:GLN:HE22	1.83	0.43
1:H:172:ASN:O	1:H:172:ASN:ND2	2.51	0.43
1:I:160:ASN:HD22	1:I:185:ASN:HA	1.83	0.43
1:S:160:ASN:HD22	1:S:185:ASN:HA	1.83	0.43
1:T:172:ASN:O	1:T:172:ASN:ND2	2.51	0.43
1:V:150:VAL:HG12	1:V:165:GLY:HA3	1.99	0.43
1:W:172:ASN:O	1:W:172:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:172:ASN:O	1:Y:172:ASN:ND2	2.51	0.43
1:H:160:ASN:HD22	1:H:185:ASN:HA	1.84	0.43
1:L:160:ASN:HD22	1:L:185:ASN:HA	1.83	0.43
1:N:150:VAL:HG12	1:N:165:GLY:HA3	1.99	0.43
1:O:150:VAL:HG12	1:O:165:GLY:HA3	1.99	0.43
1:Q:160:ASN:HD22	1:Q:185:ASN:HA	1.84	0.43
1:R:150:VAL:HG12	1:R:165:GLY:HA3	1.99	0.43
1:R:160:ASN:HD22	1:R:185:ASN:HA	1.84	0.43
1:R:172:ASN:O	1:R:172:ASN:ND2	2.51	0.43
1:T:160:ASN:HD22	1:T:185:ASN:HA	1.83	0.43
1:W:28:LYS:HE2	1:W:32:GLN:HE22	1.83	0.43
1:E:22:CYS:HB2	3:E:301:OCA:H21	1.62	0.43
1:J:160:ASN:HD22	1:J:185:ASN:HA	1.83	0.43
1:K:160:ASN:HD22	1:K:185:ASN:HA	1.83	0.43
1:L:166:GLU:OE1	1:L:168:GLN:NE2	2.32	0.43
1:M:160:ASN:HD22	1:M:185:ASN:HA	1.84	0.43
1:P:28:LYS:HE2	1:P:32:GLN:HE22	1.83	0.43
1:S:172:ASN:ND2	1:S:172:ASN:O	2.51	0.43
1:U:28:LYS:HE2	1:U:32:GLN:HE22	1.83	0.43
1:G:160:ASN:HD22	1:G:185:ASN:HA	1.83	0.43
1:G:172:ASN:ND2	1:G:172:ASN:O	2.51	0.43
1:U:150:VAL:HG12	1:U:165:GLY:HA3	1.99	0.43
1:U:160:ASN:HD22	1:U:185:ASN:HA	1.83	0.43
1:C:28:LYS:HE2	1:C:32:GLN:HE22	1.83	0.43
1:M:28:LYS:HE2	1:M:32:GLN:HE22	1.83	0.43
1:Q:172:ASN:ND2	1:Q:172:ASN:O	2.51	0.43
1:Z:160:ASN:HD22	1:Z:185:ASN:HA	1.83	0.43
1:A:132:PHE:CD1	1:C:219:MET:HG2	2.53	0.43
1:D:185:ASN:O	1:D:188:THR:OG1	2.33	0.43
1:F:172:ASN:O	1:F:172:ASN:ND2	2.51	0.43
1:M:172:ASN:O	1:M:172:ASN:ND2	2.51	0.43
1:T:150:VAL:HG12	1:T:165:GLY:HA3	1.99	0.43
1:U:185:ASN:O	1:U:188:THR:OG1	2.33	0.43
1:Y:160:ASN:HD22	1:Y:185:ASN:HA	1.83	0.43
1:E:166:GLU:OE1	1:E:168:GLN:NE2	2.32	0.43
1:H:28:LYS:HE2	1:H:32:GLN:HE22	1.83	0.43
1:K:172:ASN:O	1:K:172:ASN:ND2	2.51	0.43
1:L:28:LYS:HE2	1:L:32:GLN:HE22	1.83	0.43
1:S:150:VAL:HG12	1:S:165:GLY:HA3	1.99	0.43
1:V:160:ASN:HD22	1:V:185:ASN:HA	1.83	0.43
1:A:160:ASN:HD22	1:A:185:ASN:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:HE2	1:B:32:GLN:HE22	1.83	0.43
1:N:172:ASN:ND2	1:N:172:ASN:O	2.51	0.43
1:O:172:ASN:O	1:O:172:ASN:ND2	2.51	0.43
1:V:22:CYS:HB2	3:V:301:OCA:H21	1.63	0.43
1:X:160:ASN:HD22	1:X:185:ASN:HA	1.83	0.43
1:G:28:LYS:HE2	1:G:32:GLN:HE22	1.83	0.43
1:I:172:ASN:ND2	1:I:172:ASN:O	2.51	0.43
1:Q:28:LYS:HE2	1:Q:32:GLN:HE22	1.83	0.43
1:T:28:LYS:HE2	1:T:32:GLN:HE22	1.83	0.43
1:B:160:ASN:HD22	1:B:185:ASN:HA	1.83	0.43
1:J:172:ASN:O	1:J:172:ASN:ND2	2.51	0.43
1:L:22:CYS:HB2	3:L:301:OCA:H21	1.63	0.43
1:L:172:ASN:ND2	1:L:172:ASN:O	2.51	0.43
1:R:166:GLU:OE1	1:R:168:GLN:NE2	2.32	0.43
1:W:160:ASN:HD22	1:W:185:ASN:HA	1.83	0.43
1:F:160:ASN:HD22	1:F:185:ASN:HA	1.84	0.42
1:H:224:ARG:O	1:H:228:ASN:ND2	2.50	0.42
1:I:185:ASN:O	1:I:188:THR:OG1	2.33	0.42
1:K:166:GLU:OE1	1:K:168:GLN:NE2	2.32	0.42
1:T:107:ASP:HB3	1:U:125:GLU:HG2	2.00	0.42
1:X:28:LYS:HE2	1:X:32:GLN:HE22	1.83	0.42
1:M:224:ARG:O	1:M:228:ASN:ND2	2.50	0.42
1:I:22:CYS:HB2	3:I:301:OCA:H21	1.63	0.42
1:V:107:ASP:HB3	1:W:125:GLU:HG2	2.01	0.42
1:W:22:CYS:HB2	3:W:301:OCA:H21	1.63	0.42
1:Y:22:CYS:HB2	3:Y:301:OCA:H21	1.63	0.42
1:F:166:GLU:OE1	1:F:168:GLN:NE2	2.32	0.42
1:P:172:ASN:O	1:P:172:ASN:ND2	2.51	0.42
1:C:160:ASN:HD22	1:C:185:ASN:HA	1.83	0.42
1:E:107:ASP:HB3	1:F:125:GLU:HG2	2.01	0.42
1:X:22:CYS:HB2	3:X:301:OCA:H21	1.63	0.42
1:I:224:ARG:O	1:I:228:ASN:ND2	2.50	0.42
1:J:166:GLU:OE1	1:J:168:GLN:NE2	2.32	0.42
1:E:160:ASN:HD22	1:E:185:ASN:HA	1.83	0.42
1:L:107:ASP:HB3	1:M:125:GLU:HG2	2.01	0.42
1:Q:22:CYS:HB2	3:Q:301:OCA:H21	1.63	0.42
1:L:224:ARG:O	1:L:228:ASN:ND2	2.50	0.42
1:G:166:GLU:OE1	1:G:168:GLN:NE2	2.32	0.42
1:N:107:ASP:HB3	1:O:125:GLU:HG2	2.01	0.42
1:D:160:ASN:HD22	1:D:185:ASN:HA	1.83	0.42
1:I:166:GLU:OE1	1:I:168:GLN:NE2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:107:ASP:HB3	1:S:125:GLU:HG2	2.02	0.42
1:C:185:ASN:O	1:C:188:THR:OG1	2.33	0.41
1:H:166:GLU:OE1	1:H:168:GLN:NE2	2.32	0.41
1:J:224:ARG:O	1:J:228:ASN:ND2	2.50	0.41
1:D:107:ASP:HB3	1:E:125:GLU:HG2	2.03	0.41
1:Q:107:ASP:HB3	1:R:125:GLU:HG2	2.01	0.41
1:Q:166:GLU:OE1	1:Q:168:GLN:NE2	2.32	0.41
1:K:224:ARG:O	1:K:228:ASN:ND2	2.50	0.41
1:E:224:ARG:O	1:E:228:ASN:ND2	2.50	0.41
1:H:185:ASN:O	1:H:188:THR:OG1	2.33	0.41
1:A:125:GLU:HG2	1:Z:107:ASP:HB3	2.03	0.41
1:G:107:ASP:HB3	1:H:125:GLU:HG2	2.03	0.41
1:I:107:ASP:HB3	1:J:125:GLU:HG2	2.02	0.41
1:P:107:ASP:HB3	1:Q:125:GLU:HG2	2.02	0.41
1:A:107:ASP:HB3	1:B:125:GLU:HG2	2.04	0.40
1:F:22:CYS:HB2	3:F:301:OCA:H21	1.63	0.40
1:N:45:PRO:HB3	1:N:53:GLN:HG3	2.04	0.40
1:J:107:ASP:HB3	1:K:125:GLU:HG2	2.03	0.40
1:O:45:PRO:HB3	1:O:53:GLN:HG3	2.04	0.40
1:W:45:PRO:HB3	1:W:53:GLN:HG3	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%)	199 (95%)	10 (5%)	0	100	100
1	B	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	C	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	D	209/232 (90%)	199 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	F	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	G	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	H	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	I	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	J	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	K	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	L	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	M	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	N	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	O	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	P	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	Q	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	R	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	S	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	T	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	U	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	V	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	W	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	X	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
1	Y	209/232 (90%)	198 (95%)	11 (5%)	0	100	100
1	Z	209/232 (90%)	199 (95%)	10 (5%)	0	100	100
2	a	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	b	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	c	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	d	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	e	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	f	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	g	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	h	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	i	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	j	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	k	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	l	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	m	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	n	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	o	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	p	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	q	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	r	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	s	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	t	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	u	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	v	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	w	297/365 (81%)	290 (98%)	6 (2%)	1 (0%)	41	72
2	x	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	y	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
2	z	297/365 (81%)	291 (98%)	5 (2%)	1 (0%)	41	72
All	All	13156/15522 (85%)	12738 (97%)	392 (3%)	26 (0%)	50	78

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	112	ASN
2	b	112	ASN
2	c	112	ASN
2	d	112	ASN
2	e	112	ASN
2	f	112	ASN
2	g	112	ASN
2	h	112	ASN
2	i	112	ASN
2	j	112	ASN
2	k	112	ASN
2	l	112	ASN
2	m	112	ASN
2	n	112	ASN

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Mol	Chain	Res	Type
2	o	112	ASN
2	p	112	ASN
2	q	112	ASN
2	r	112	ASN
2	s	112	ASN
2	t	112	ASN
2	u	112	ASN
2	v	112	ASN
2	w	112	ASN
2	x	112	ASN
2	y	112	ASN
2	z	112	ASN

### 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	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	B	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	C	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	D	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	E	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	F	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	G	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	H	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	I	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	J	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	K	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	L	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	M	170/186 (91%)	159 (94%)	11 (6%)	17 44
1	N	170/186 (91%)	159 (94%)	11 (6%)	17 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	P	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	Q	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	R	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	S	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	T	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	U	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	V	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	W	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	X	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	Y	170/186 (91%)	159 (94%)	11 (6%)	17	44
1	Z	170/186 (91%)	159 (94%)	11 (6%)	17	44
2	a	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	b	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	c	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	d	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	e	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	f	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	g	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	h	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	i	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	j	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	k	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	l	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	m	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	n	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	o	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	p	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	q	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	r	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	s	248/294 (84%)	237 (96%)	11 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	t	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	u	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	v	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	w	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	x	248/294 (84%)	237 (96%)	11 (4%)	28	61
2	y	248/294 (84%)	236 (95%)	12 (5%)	25	58
2	z	248/294 (84%)	237 (96%)	11 (4%)	28	61
All	All	10868/12480 (87%)	10284 (95%)	584 (5%)	26	53

All (584) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	89	SER
1	A	103	SER
1	A	106	PHE
1	A	127	SER
1	A	131	SER
1	A	141	SER
1	A	143	THR
1	A	144	PHE
1	A	145	SER
1	A	194	SER
1	B	40	ILE
1	B	89	SER
1	B	103	SER
1	B	106	PHE
1	B	127	SER
1	B	131	SER
1	B	141	SER
1	B	143	THR
1	B	144	PHE
1	B	145	SER
1	B	194	SER
1	C	40	ILE
1	C	89	SER
1	C	103	SER
1	C	106	PHE
1	C	127	SER
1	C	131	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	141	SER
1	C	143	THR
1	C	144	PHE
1	C	145	SER
1	C	194	SER
1	D	40	ILE
1	D	89	SER
1	D	103	SER
1	D	106	PHE
1	D	127	SER
1	D	131	SER
1	D	141	SER
1	D	143	THR
1	D	144	PHE
1	D	145	SER
1	D	194	SER
1	E	40	ILE
1	E	89	SER
1	E	103	SER
1	E	106	PHE
1	E	127	SER
1	E	131	SER
1	E	141	SER
1	E	143	THR
1	E	144	PHE
1	E	145	SER
1	E	194	SER
1	F	40	ILE
1	F	89	SER
1	F	103	SER
1	F	106	PHE
1	F	127	SER
1	F	131	SER
1	F	141	SER
1	F	143	THR
1	F	144	PHE
1	F	145	SER
1	F	194	SER
1	G	40	ILE
1	G	89	SER
1	G	103	SER
1	G	106	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	127	SER
1	G	131	SER
1	G	141	SER
1	G	143	THR
1	G	144	PHE
1	G	145	SER
1	G	194	SER
1	H	40	ILE
1	H	89	SER
1	H	103	SER
1	H	106	PHE
1	H	127	SER
1	H	131	SER
1	H	141	SER
1	H	143	THR
1	H	144	PHE
1	H	145	SER
1	H	194	SER
1	I	40	ILE
1	I	89	SER
1	I	103	SER
1	I	106	PHE
1	I	127	SER
1	I	131	SER
1	I	141	SER
1	I	143	THR
1	I	144	PHE
1	I	145	SER
1	I	194	SER
1	J	40	ILE
1	J	89	SER
1	J	103	SER
1	J	106	PHE
1	J	127	SER
1	J	131	SER
1	J	141	SER
1	J	143	THR
1	J	144	PHE
1	J	145	SER
1	J	194	SER
1	K	40	ILE
1	K	89	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	103	SER
1	K	106	PHE
1	K	127	SER
1	K	131	SER
1	K	141	SER
1	K	143	THR
1	K	144	PHE
1	K	145	SER
1	K	194	SER
1	L	40	ILE
1	L	89	SER
1	L	103	SER
1	L	106	PHE
1	L	127	SER
1	L	131	SER
1	L	141	SER
1	L	143	THR
1	L	144	PHE
1	L	145	SER
1	L	194	SER
1	M	40	ILE
1	M	89	SER
1	M	103	SER
1	M	106	PHE
1	M	127	SER
1	M	131	SER
1	M	141	SER
1	M	143	THR
1	M	144	PHE
1	M	145	SER
1	M	194	SER
1	N	40	ILE
1	N	89	SER
1	N	103	SER
1	N	106	PHE
1	N	127	SER
1	N	131	SER
1	N	141	SER
1	N	143	THR
1	N	144	PHE
1	N	145	SER
1	N	194	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	40	ILE
1	O	89	SER
1	O	103	SER
1	O	106	PHE
1	O	127	SER
1	O	131	SER
1	O	141	SER
1	O	143	THR
1	O	144	PHE
1	O	145	SER
1	O	194	SER
1	P	40	ILE
1	P	89	SER
1	P	103	SER
1	P	106	PHE
1	P	127	SER
1	P	131	SER
1	P	141	SER
1	P	143	THR
1	P	144	PHE
1	P	145	SER
1	P	194	SER
1	Q	40	ILE
1	Q	89	SER
1	Q	103	SER
1	Q	106	PHE
1	Q	127	SER
1	Q	131	SER
1	Q	141	SER
1	Q	143	THR
1	Q	144	PHE
1	Q	145	SER
1	Q	194	SER
1	R	40	ILE
1	R	89	SER
1	R	103	SER
1	R	106	PHE
1	R	127	SER
1	R	131	SER
1	R	141	SER
1	R	143	THR
1	R	144	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	R	145	SER
1	R	194	SER
1	S	40	ILE
1	S	89	SER
1	S	103	SER
1	S	106	PHE
1	S	127	SER
1	S	131	SER
1	S	141	SER
1	S	143	THR
1	S	144	PHE
1	S	145	SER
1	S	194	SER
1	T	40	ILE
1	T	89	SER
1	T	103	SER
1	T	106	PHE
1	T	127	SER
1	T	131	SER
1	T	141	SER
1	T	143	THR
1	T	144	PHE
1	T	145	SER
1	T	194	SER
1	U	40	ILE
1	U	89	SER
1	U	103	SER
1	U	106	PHE
1	U	127	SER
1	U	131	SER
1	U	141	SER
1	U	143	THR
1	U	144	PHE
1	U	145	SER
1	U	194	SER
1	V	40	ILE
1	V	89	SER
1	V	103	SER
1	V	106	PHE
1	V	127	SER
1	V	131	SER
1	V	141	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	V	143	THR
1	V	144	PHE
1	V	145	SER
1	V	194	SER
1	W	40	ILE
1	W	89	SER
1	W	103	SER
1	W	106	PHE
1	W	127	SER
1	W	131	SER
1	W	141	SER
1	W	143	THR
1	W	144	PHE
1	W	145	SER
1	W	194	SER
1	X	40	ILE
1	X	89	SER
1	X	103	SER
1	X	106	PHE
1	X	127	SER
1	X	131	SER
1	X	141	SER
1	X	143	THR
1	X	144	PHE
1	X	145	SER
1	X	194	SER
1	Y	40	ILE
1	Y	89	SER
1	Y	103	SER
1	Y	106	PHE
1	Y	127	SER
1	Y	131	SER
1	Y	141	SER
1	Y	143	THR
1	Y	144	PHE
1	Y	145	SER
1	Y	194	SER
1	Z	40	ILE
1	Z	89	SER
1	Z	103	SER
1	Z	106	PHE
1	Z	127	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Z	131	SER
1	Z	141	SER
1	Z	143	THR
1	Z	144	PHE
1	Z	145	SER
1	Z	194	SER
2	a	21	ARG
2	a	23	ARG
2	a	27	SER
2	a	53	THR
2	a	75	THR
2	a	191	ASP
2	a	220	THR
2	a	231	SER
2	a	250	ASP
2	a	281	SER
2	a	321	SER
2	a	344	ASP
2	b	21	ARG
2	b	23	ARG
2	b	27	SER
2	b	53	THR
2	b	75	THR
2	b	191	ASP
2	b	220	THR
2	b	231	SER
2	b	281	SER
2	b	321	SER
2	b	344	ASP
2	c	21	ARG
2	c	23	ARG
2	c	27	SER
2	c	53	THR
2	c	75	THR
2	c	191	ASP
2	c	220	THR
2	c	231	SER
2	c	250	ASP
2	c	281	SER
2	c	321	SER
2	c	344	ASP
2	d	21	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	d	23	ARG
2	d	27	SER
2	d	53	THR
2	d	75	THR
2	d	191	ASP
2	d	220	THR
2	d	231	SER
2	d	281	SER
2	d	321	SER
2	d	344	ASP
2	e	21	ARG
2	e	23	ARG
2	e	27	SER
2	e	53	THR
2	e	75	THR
2	e	191	ASP
2	e	220	THR
2	e	231	SER
2	e	250	ASP
2	e	281	SER
2	e	321	SER
2	e	344	ASP
2	f	21	ARG
2	f	23	ARG
2	f	27	SER
2	f	53	THR
2	f	75	THR
2	f	191	ASP
2	f	220	THR
2	f	231	SER
2	f	281	SER
2	f	321	SER
2	f	344	ASP
2	g	21	ARG
2	g	23	ARG
2	g	27	SER
2	g	53	THR
2	g	75	THR
2	g	191	ASP
2	g	220	THR
2	g	231	SER
2	g	250	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	g	281	SER
2	g	321	SER
2	g	344	ASP
2	h	21	ARG
2	h	23	ARG
2	h	27	SER
2	h	53	THR
2	h	75	THR
2	h	191	ASP
2	h	220	THR
2	h	231	SER
2	h	250	ASP
2	h	281	SER
2	h	321	SER
2	h	344	ASP
2	i	21	ARG
2	i	23	ARG
2	i	27	SER
2	i	53	THR
2	i	75	THR
2	i	191	ASP
2	i	220	THR
2	i	231	SER
2	i	281	SER
2	i	321	SER
2	i	344	ASP
2	j	21	ARG
2	j	23	ARG
2	j	27	SER
2	j	53	THR
2	j	75	THR
2	j	191	ASP
2	j	220	THR
2	j	231	SER
2	j	281	SER
2	j	321	SER
2	j	344	ASP
2	k	21	ARG
2	k	23	ARG
2	k	27	SER
2	k	53	THR
2	k	75	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	k	191	ASP
2	k	220	THR
2	k	231	SER
2	k	250	ASP
2	k	281	SER
2	k	321	SER
2	k	344	ASP
2	l	21	ARG
2	l	23	ARG
2	l	27	SER
2	l	53	THR
2	l	75	THR
2	l	191	ASP
2	l	220	THR
2	l	231	SER
2	l	281	SER
2	l	321	SER
2	l	344	ASP
2	m	21	ARG
2	m	23	ARG
2	m	27	SER
2	m	53	THR
2	m	75	THR
2	m	191	ASP
2	m	220	THR
2	m	231	SER
2	m	250	ASP
2	m	281	SER
2	m	321	SER
2	m	344	ASP
2	n	21	ARG
2	n	23	ARG
2	n	27	SER
2	n	53	THR
2	n	75	THR
2	n	191	ASP
2	n	220	THR
2	n	231	SER
2	n	281	SER
2	n	321	SER
2	n	344	ASP
2	o	21	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	o	23	ARG
2	o	27	SER
2	o	53	THR
2	o	75	THR
2	o	191	ASP
2	o	220	THR
2	o	231	SER
2	o	281	SER
2	o	321	SER
2	o	344	ASP
2	p	21	ARG
2	p	23	ARG
2	p	27	SER
2	p	53	THR
2	p	75	THR
2	p	191	ASP
2	p	220	THR
2	p	231	SER
2	p	250	ASP
2	p	281	SER
2	p	321	SER
2	p	344	ASP
2	q	21	ARG
2	q	23	ARG
2	q	27	SER
2	q	53	THR
2	q	75	THR
2	q	191	ASP
2	q	220	THR
2	q	231	SER
2	q	281	SER
2	q	321	SER
2	q	344	ASP
2	r	21	ARG
2	r	23	ARG
2	r	27	SER
2	r	53	THR
2	r	75	THR
2	r	191	ASP
2	r	220	THR
2	r	231	SER
2	r	250	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	r	281	SER
2	r	321	SER
2	r	344	ASP
2	s	21	ARG
2	s	23	ARG
2	s	27	SER
2	s	53	THR
2	s	75	THR
2	s	191	ASP
2	s	220	THR
2	s	231	SER
2	s	281	SER
2	s	321	SER
2	s	344	ASP
2	t	21	ARG
2	t	23	ARG
2	t	27	SER
2	t	53	THR
2	t	75	THR
2	t	191	ASP
2	t	220	THR
2	t	231	SER
2	t	250	ASP
2	t	281	SER
2	t	321	SER
2	t	344	ASP
2	u	21	ARG
2	u	23	ARG
2	u	27	SER
2	u	53	THR
2	u	75	THR
2	u	191	ASP
2	u	220	THR
2	u	231	SER
2	u	250	ASP
2	u	281	SER
2	u	321	SER
2	u	344	ASP
2	v	21	ARG
2	v	23	ARG
2	v	27	SER
2	v	53	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	v	75	THR
2	v	191	ASP
2	v	220	THR
2	v	231	SER
2	v	281	SER
2	v	321	SER
2	v	344	ASP
2	w	21	ARG
2	w	23	ARG
2	w	27	SER
2	w	53	THR
2	w	75	THR
2	w	191	ASP
2	w	220	THR
2	w	231	SER
2	w	281	SER
2	w	321	SER
2	w	344	ASP
2	x	21	ARG
2	x	23	ARG
2	x	27	SER
2	x	53	THR
2	x	75	THR
2	x	191	ASP
2	x	220	THR
2	x	231	SER
2	x	281	SER
2	x	321	SER
2	x	344	ASP
2	y	21	ARG
2	y	23	ARG
2	y	27	SER
2	y	53	THR
2	y	75	THR
2	y	191	ASP
2	y	220	THR
2	y	231	SER
2	y	250	ASP
2	y	281	SER
2	y	321	SER
2	y	344	ASP
2	z	21	ARG

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Mol	Chain	Res	Type
2	z	23	ARG
2	z	27	SER
2	z	53	THR
2	z	75	THR
2	z	191	ASP
2	z	220	THR
2	z	231	SER
2	z	281	SER
2	z	321	SER
2	z	344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (378) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	114	GLN
1	A	119	ASN
1	A	133	ASN
1	A	172	ASN
1	A	217	GLN
1	B	63	GLN
1	B	114	GLN
1	B	119	ASN
1	B	133	ASN
1	B	172	ASN
1	B	217	GLN
1	C	63	GLN
1	C	83	GLN
1	C	114	GLN
1	C	119	ASN
1	C	133	ASN
1	C	172	ASN
1	C	217	GLN
1	D	63	GLN
1	D	114	GLN
1	D	119	ASN
1	D	133	ASN
1	D	172	ASN
1	D	217	GLN
1	E	63	GLN
1	E	83	GLN
1	E	114	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	119	ASN
1	E	133	ASN
1	E	172	ASN
1	E	217	GLN
1	F	63	GLN
1	F	114	GLN
1	F	119	ASN
1	F	133	ASN
1	F	172	ASN
1	F	217	GLN
1	G	63	GLN
1	G	114	GLN
1	G	119	ASN
1	G	133	ASN
1	G	172	ASN
1	G	217	GLN
1	H	63	GLN
1	H	83	GLN
1	H	114	GLN
1	H	119	ASN
1	H	133	ASN
1	H	172	ASN
1	H	217	GLN
1	I	63	GLN
1	I	114	GLN
1	I	119	ASN
1	I	133	ASN
1	I	172	ASN
1	I	217	GLN
1	J	63	GLN
1	J	83	GLN
1	J	114	GLN
1	J	119	ASN
1	J	133	ASN
1	J	172	ASN
1	J	217	GLN
1	K	63	GLN
1	K	114	GLN
1	K	119	ASN
1	K	133	ASN
1	K	172	ASN
1	K	217	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	63	GLN
1	L	114	GLN
1	L	119	ASN
1	L	133	ASN
1	L	172	ASN
1	L	217	GLN
1	M	63	GLN
1	M	114	GLN
1	M	119	ASN
1	M	133	ASN
1	M	172	ASN
1	M	217	GLN
1	N	63	GLN
1	N	114	GLN
1	N	119	ASN
1	N	133	ASN
1	N	172	ASN
1	N	217	GLN
1	O	63	GLN
1	O	114	GLN
1	O	119	ASN
1	O	133	ASN
1	O	172	ASN
1	O	217	GLN
1	P	63	GLN
1	P	83	GLN
1	P	114	GLN
1	P	119	ASN
1	P	133	ASN
1	P	172	ASN
1	P	217	GLN
1	Q	63	GLN
1	Q	83	GLN
1	Q	114	GLN
1	Q	119	ASN
1	Q	133	ASN
1	Q	172	ASN
1	Q	217	GLN
1	R	63	GLN
1	R	83	GLN
1	R	114	GLN
1	R	119	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	R	133	ASN
1	R	172	ASN
1	R	217	GLN
1	S	63	GLN
1	S	83	GLN
1	S	114	GLN
1	S	119	ASN
1	S	133	ASN
1	S	172	ASN
1	S	217	GLN
1	T	63	GLN
1	T	83	GLN
1	T	114	GLN
1	T	119	ASN
1	T	133	ASN
1	T	172	ASN
1	T	217	GLN
1	U	63	GLN
1	U	114	GLN
1	U	119	ASN
1	U	133	ASN
1	U	172	ASN
1	U	217	GLN
1	V	63	GLN
1	V	114	GLN
1	V	119	ASN
1	V	133	ASN
1	V	172	ASN
1	V	217	GLN
1	W	63	GLN
1	W	83	GLN
1	W	114	GLN
1	W	119	ASN
1	W	133	ASN
1	W	172	ASN
1	W	217	GLN
1	X	63	GLN
1	X	114	GLN
1	X	119	ASN
1	X	133	ASN
1	X	172	ASN
1	X	217	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Y	63	GLN
1	Y	114	GLN
1	Y	119	ASN
1	Y	133	ASN
1	Y	172	ASN
1	Y	217	GLN
1	Z	63	GLN
1	Z	114	GLN
1	Z	119	ASN
1	Z	133	ASN
1	Z	172	ASN
1	Z	217	GLN
2	a	54	GLN
2	a	80	GLN
2	a	159	GLN
2	a	161	ASN
2	a	188	GLN
2	a	198	GLN
2	a	277	GLN
2	b	54	GLN
2	b	68	GLN
2	b	80	GLN
2	b	159	GLN
2	b	161	ASN
2	b	188	GLN
2	b	198	GLN
2	b	277	GLN
2	c	54	GLN
2	c	68	GLN
2	c	80	GLN
2	c	159	GLN
2	c	161	ASN
2	c	188	GLN
2	c	198	GLN
2	c	277	GLN
2	d	54	GLN
2	d	68	GLN
2	d	80	GLN
2	d	159	GLN
2	d	161	ASN
2	d	188	GLN
2	d	198	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	d	241	ASN
2	d	277	GLN
2	e	54	GLN
2	e	68	GLN
2	e	80	GLN
2	e	159	GLN
2	e	161	ASN
2	e	188	GLN
2	e	198	GLN
2	e	277	GLN
2	f	54	GLN
2	f	68	GLN
2	f	80	GLN
2	f	159	GLN
2	f	161	ASN
2	f	188	GLN
2	f	198	GLN
2	f	277	GLN
2	g	54	GLN
2	g	68	GLN
2	g	80	GLN
2	g	159	GLN
2	g	161	ASN
2	g	188	GLN
2	g	198	GLN
2	g	277	GLN
2	h	54	GLN
2	h	68	GLN
2	h	80	GLN
2	h	159	GLN
2	h	161	ASN
2	h	188	GLN
2	h	198	GLN
2	h	277	GLN
2	i	54	GLN
2	i	68	GLN
2	i	80	GLN
2	i	159	GLN
2	i	161	ASN
2	i	188	GLN
2	i	198	GLN
2	i	277	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	j	54	GLN
2	j	68	GLN
2	j	80	GLN
2	j	159	GLN
2	j	161	ASN
2	j	188	GLN
2	j	198	GLN
2	j	277	GLN
2	k	54	GLN
2	k	68	GLN
2	k	80	GLN
2	k	159	GLN
2	k	161	ASN
2	k	188	GLN
2	k	198	GLN
2	k	277	GLN
2	l	54	GLN
2	l	68	GLN
2	l	80	GLN
2	l	159	GLN
2	l	161	ASN
2	l	188	GLN
2	l	198	GLN
2	l	241	ASN
2	l	277	GLN
2	m	54	GLN
2	m	68	GLN
2	m	80	GLN
2	m	159	GLN
2	m	161	ASN
2	m	188	GLN
2	m	198	GLN
2	m	241	ASN
2	m	277	GLN
2	n	54	GLN
2	n	68	GLN
2	n	80	GLN
2	n	159	GLN
2	n	188	GLN
2	n	198	GLN
2	n	241	ASN
2	n	277	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	o	54	GLN
2	o	68	GLN
2	o	80	GLN
2	o	159	GLN
2	o	161	ASN
2	o	188	GLN
2	o	198	GLN
2	o	277	GLN
2	p	54	GLN
2	p	68	GLN
2	p	80	GLN
2	p	159	GLN
2	p	161	ASN
2	p	188	GLN
2	p	198	GLN
2	p	277	GLN
2	q	54	GLN
2	q	68	GLN
2	q	80	GLN
2	q	159	GLN
2	q	161	ASN
2	q	188	GLN
2	q	198	GLN
2	q	277	GLN
2	r	54	GLN
2	r	68	GLN
2	r	80	GLN
2	r	159	GLN
2	r	161	ASN
2	r	188	GLN
2	r	198	GLN
2	r	277	GLN
2	s	54	GLN
2	s	68	GLN
2	s	80	GLN
2	s	159	GLN
2	s	161	ASN
2	s	188	GLN
2	s	198	GLN
2	s	241	ASN
2	s	277	GLN
2	t	54	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	t	68	GLN
2	t	80	GLN
2	t	159	GLN
2	t	161	ASN
2	t	188	GLN
2	t	198	GLN
2	t	241	ASN
2	t	277	GLN
2	u	54	GLN
2	u	68	GLN
2	u	80	GLN
2	u	159	GLN
2	u	161	ASN
2	u	188	GLN
2	u	198	GLN
2	u	241	ASN
2	u	277	GLN
2	v	54	GLN
2	v	68	GLN
2	v	80	GLN
2	v	159	GLN
2	v	161	ASN
2	v	188	GLN
2	v	198	GLN
2	w	54	GLN
2	w	68	GLN
2	w	80	GLN
2	w	159	GLN
2	w	161	ASN
2	w	188	GLN
2	w	198	GLN
2	w	277	GLN
2	x	54	GLN
2	x	68	GLN
2	x	80	GLN
2	x	159	GLN
2	x	161	ASN
2	x	188	GLN
2	x	198	GLN
2	x	277	GLN
2	y	54	GLN
2	y	68	GLN

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Mol	Chain	Res	Type
2	y	80	GLN
2	y	159	GLN
2	y	161	ASN
2	y	188	GLN
2	y	198	GLN
2	y	277	GLN
2	z	54	GLN
2	z	68	GLN
2	z	80	GLN
2	z	159	GLN
2	z	161	ASN
2	z	188	GLN
2	z	198	GLN
2	z	277	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OCA	K	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	H	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	V	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	L	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	I	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	R	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	F	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	W	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	C	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	Z	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	D	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	Q	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	S	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	U	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	J	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	T	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	Y	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	A	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	B	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	P	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	G	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	E	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	M	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	O	301	1	8,8,9	0.30	0	7,7,9	0.49	0
3	OCA	X	301	1	8,8,9	0.29	0	7,7,9	0.49	0
3	OCA	N	301	1	8,8,9	0.29	0	7,7,9	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	K	301	1	-	3/5/6/7	-
3	OCA	H	301	1	-	3/5/6/7	-
3	OCA	V	301	1	-	3/5/6/7	-
3	OCA	L	301	1	-	3/5/6/7	-
3	OCA	I	301	1	-	3/5/6/7	-
3	OCA	R	301	1	-	3/5/6/7	-
3	OCA	F	301	1	-	3/5/6/7	-
3	OCA	W	301	1	-	3/5/6/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OCA	C	301	1	-	3/5/6/7	-
3	OCA	Z	301	1	-	3/5/6/7	-
3	OCA	D	301	1	-	3/5/6/7	-
3	OCA	Q	301	1	-	3/5/6/7	-
3	OCA	S	301	1	-	3/5/6/7	-
3	OCA	U	301	1	-	3/5/6/7	-
3	OCA	J	301	1	-	3/5/6/7	-
3	OCA	T	301	1	-	3/5/6/7	-
3	OCA	Y	301	1	-	3/5/6/7	-
3	OCA	A	301	1	-	3/5/6/7	-
3	OCA	B	301	1	-	3/5/6/7	-
3	OCA	P	301	1	-	3/5/6/7	-
3	OCA	G	301	1	-	3/5/6/7	-
3	OCA	E	301	1	-	3/5/6/7	-
3	OCA	M	301	1	-	3/5/6/7	-
3	OCA	O	301	1	-	3/5/6/7	-
3	OCA	X	301	1	-	3/5/6/7	-
3	OCA	N	301	1	-	3/5/6/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	OCA	C2-C3-C4-C5
3	B	301	OCA	C2-C3-C4-C5
3	C	301	OCA	C2-C3-C4-C5
3	D	301	OCA	C2-C3-C4-C5
3	E	301	OCA	C2-C3-C4-C5
3	F	301	OCA	C2-C3-C4-C5
3	G	301	OCA	C2-C3-C4-C5
3	H	301	OCA	C2-C3-C4-C5
3	I	301	OCA	C2-C3-C4-C5
3	J	301	OCA	C2-C3-C4-C5
3	K	301	OCA	C2-C3-C4-C5
3	L	301	OCA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	N	301	OCA	C2-C3-C4-C5
3	O	301	OCA	C2-C3-C4-C5
3	P	301	OCA	C2-C3-C4-C5
3	Q	301	OCA	C2-C3-C4-C5
3	R	301	OCA	C2-C3-C4-C5
3	S	301	OCA	C2-C3-C4-C5
3	T	301	OCA	C2-C3-C4-C5
3	U	301	OCA	C2-C3-C4-C5
3	V	301	OCA	C2-C3-C4-C5
3	W	301	OCA	C2-C3-C4-C5
3	Y	301	OCA	C2-C3-C4-C5
3	M	301	OCA	C2-C3-C4-C5
3	X	301	OCA	C2-C3-C4-C5
3	Z	301	OCA	C2-C3-C4-C5
3	A	301	OCA	C4-C5-C6-C7
3	B	301	OCA	C4-C5-C6-C7
3	C	301	OCA	C4-C5-C6-C7
3	I	301	OCA	C4-C5-C6-C7
3	J	301	OCA	C4-C5-C6-C7
3	K	301	OCA	C4-C5-C6-C7
3	M	301	OCA	C4-C5-C6-C7
3	P	301	OCA	C4-C5-C6-C7
3	U	301	OCA	C4-C5-C6-C7
3	W	301	OCA	C4-C5-C6-C7
3	X	301	OCA	C4-C5-C6-C7
3	Y	301	OCA	C4-C5-C6-C7
3	Z	301	OCA	C4-C5-C6-C7
3	D	301	OCA	C4-C5-C6-C7
3	E	301	OCA	C4-C5-C6-C7
3	G	301	OCA	C4-C5-C6-C7
3	H	301	OCA	C4-C5-C6-C7
3	L	301	OCA	C4-C5-C6-C7
3	N	301	OCA	C4-C5-C6-C7
3	O	301	OCA	C4-C5-C6-C7
3	Q	301	OCA	C4-C5-C6-C7
3	R	301	OCA	C4-C5-C6-C7
3	S	301	OCA	C4-C5-C6-C7
3	T	301	OCA	C4-C5-C6-C7
3	V	301	OCA	C4-C5-C6-C7
3	F	301	OCA	C4-C5-C6-C7
3	A	301	OCA	C3-C4-C5-C6
3	B	301	OCA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	C	301	OCA	C3-C4-C5-C6
3	D	301	OCA	C3-C4-C5-C6
3	E	301	OCA	C3-C4-C5-C6
3	F	301	OCA	C3-C4-C5-C6
3	G	301	OCA	C3-C4-C5-C6
3	H	301	OCA	C3-C4-C5-C6
3	I	301	OCA	C3-C4-C5-C6
3	J	301	OCA	C3-C4-C5-C6
3	K	301	OCA	C3-C4-C5-C6
3	L	301	OCA	C3-C4-C5-C6
3	M	301	OCA	C3-C4-C5-C6
3	N	301	OCA	C3-C4-C5-C6
3	O	301	OCA	C3-C4-C5-C6
3	P	301	OCA	C3-C4-C5-C6
3	Q	301	OCA	C3-C4-C5-C6
3	R	301	OCA	C3-C4-C5-C6
3	S	301	OCA	C3-C4-C5-C6
3	T	301	OCA	C3-C4-C5-C6
3	U	301	OCA	C3-C4-C5-C6
3	V	301	OCA	C3-C4-C5-C6
3	W	301	OCA	C3-C4-C5-C6
3	X	301	OCA	C3-C4-C5-C6
3	Y	301	OCA	C3-C4-C5-C6
3	Z	301	OCA	C3-C4-C5-C6

There are no ring outliers.

19 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	301	OCA	1	0
3	V	301	OCA	1	0
3	L	301	OCA	1	0
3	I	301	OCA	1	0
3	R	301	OCA	1	0
3	F	301	OCA	1	0
3	W	301	OCA	1	0
3	Z	301	OCA	1	0
3	Q	301	OCA	1	0
3	U	301	OCA	1	0
3	T	301	OCA	1	0
3	Y	301	OCA	1	0
3	A	301	OCA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	OCA	1	0
3	P	301	OCA	1	0
3	G	301	OCA	1	0
3	E	301	OCA	1	0
3	M	301	OCA	1	0
3	X	301	OCA	1	0

## 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.

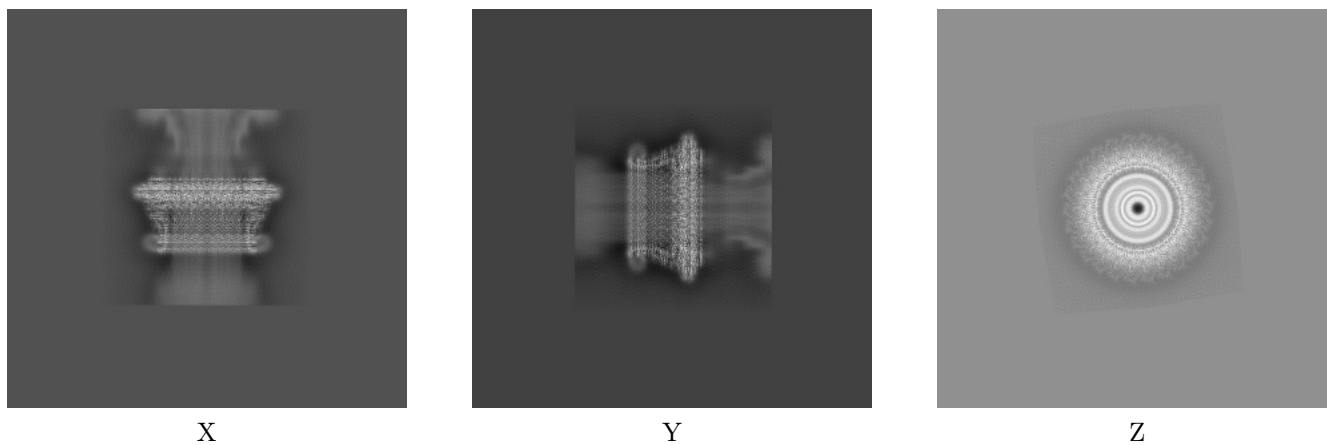
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30335. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

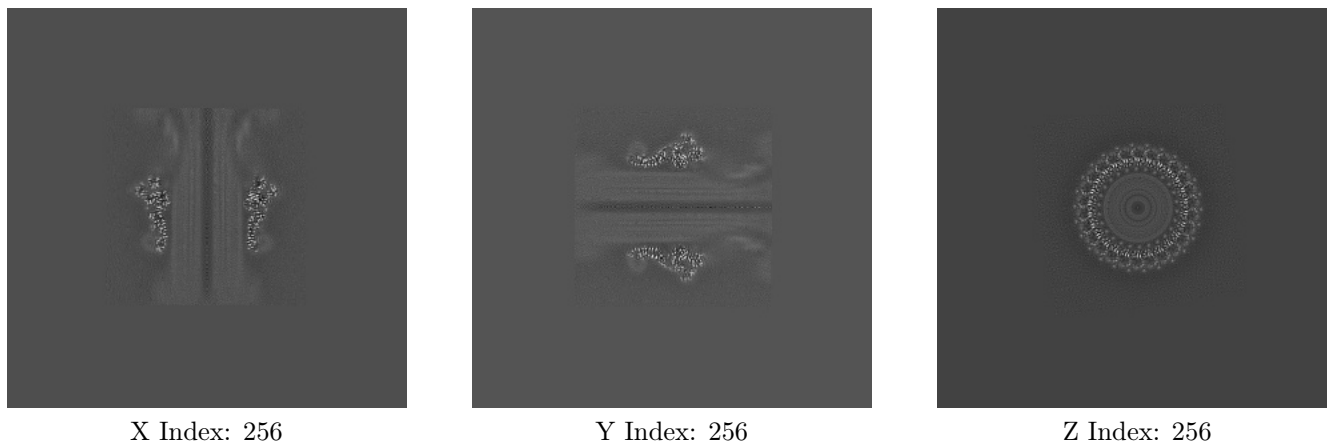
#### 6.1.1 Primary map



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

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

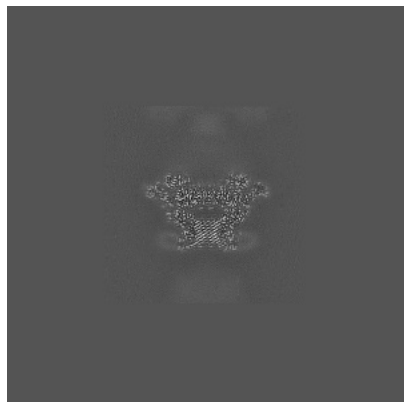
#### 6.2.1 Primary map



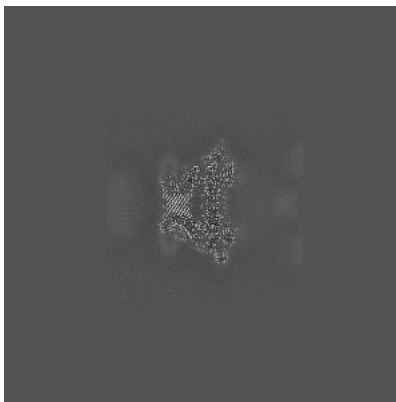
The images above show central slices of the map in three orthogonal directions.

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

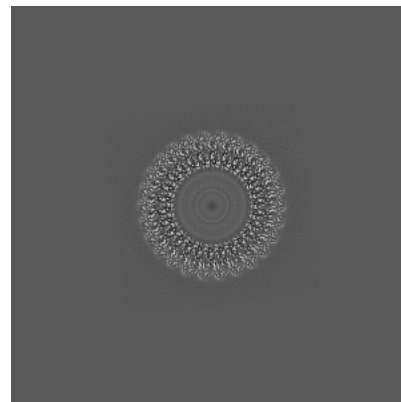
### 6.3.1 Primary map



X Index: 204



Y Index: 309



Z Index: 271

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

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

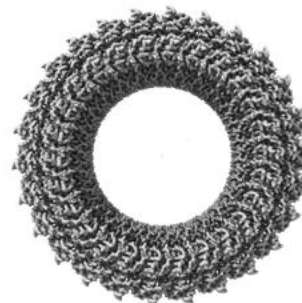
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.809. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

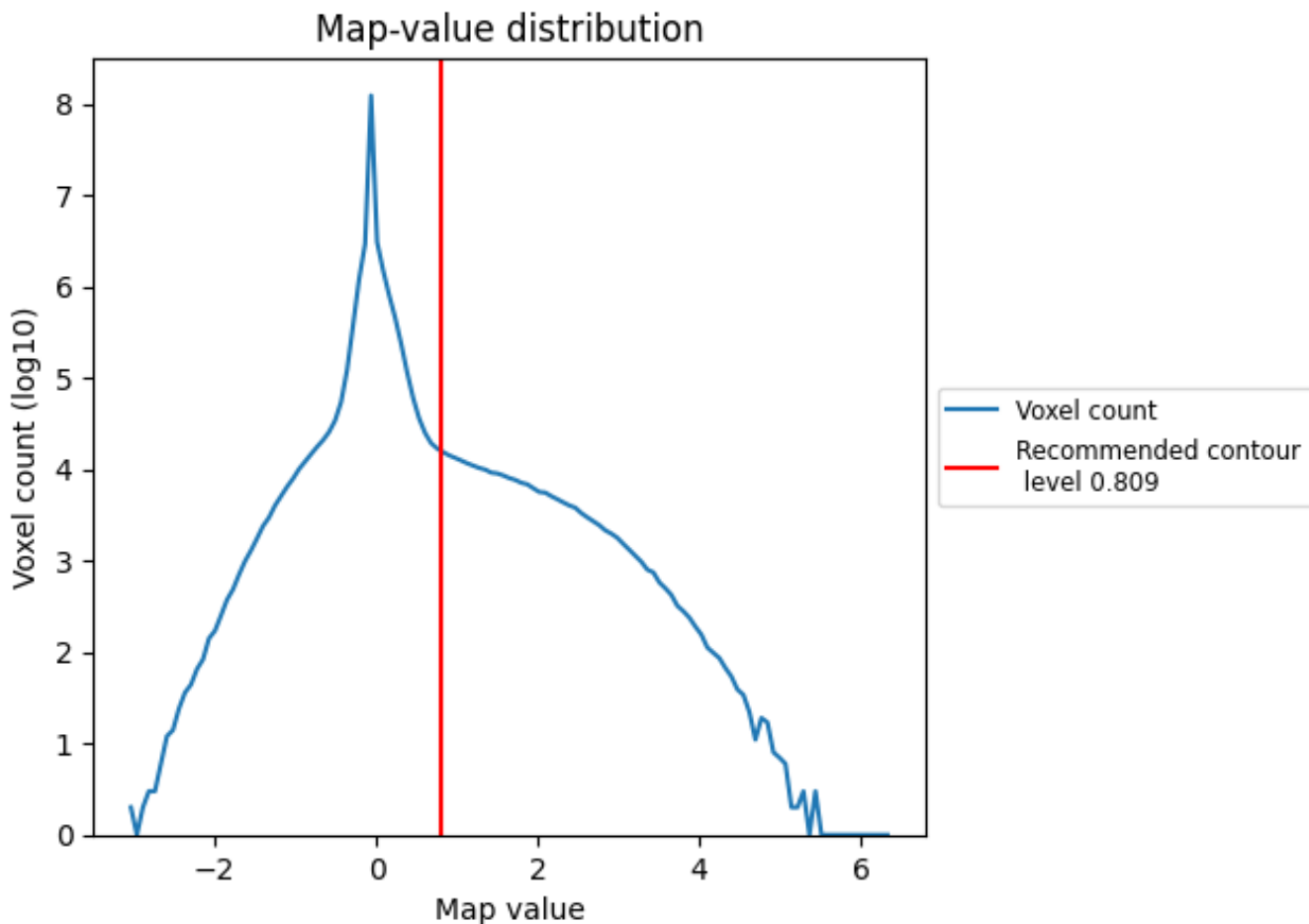
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

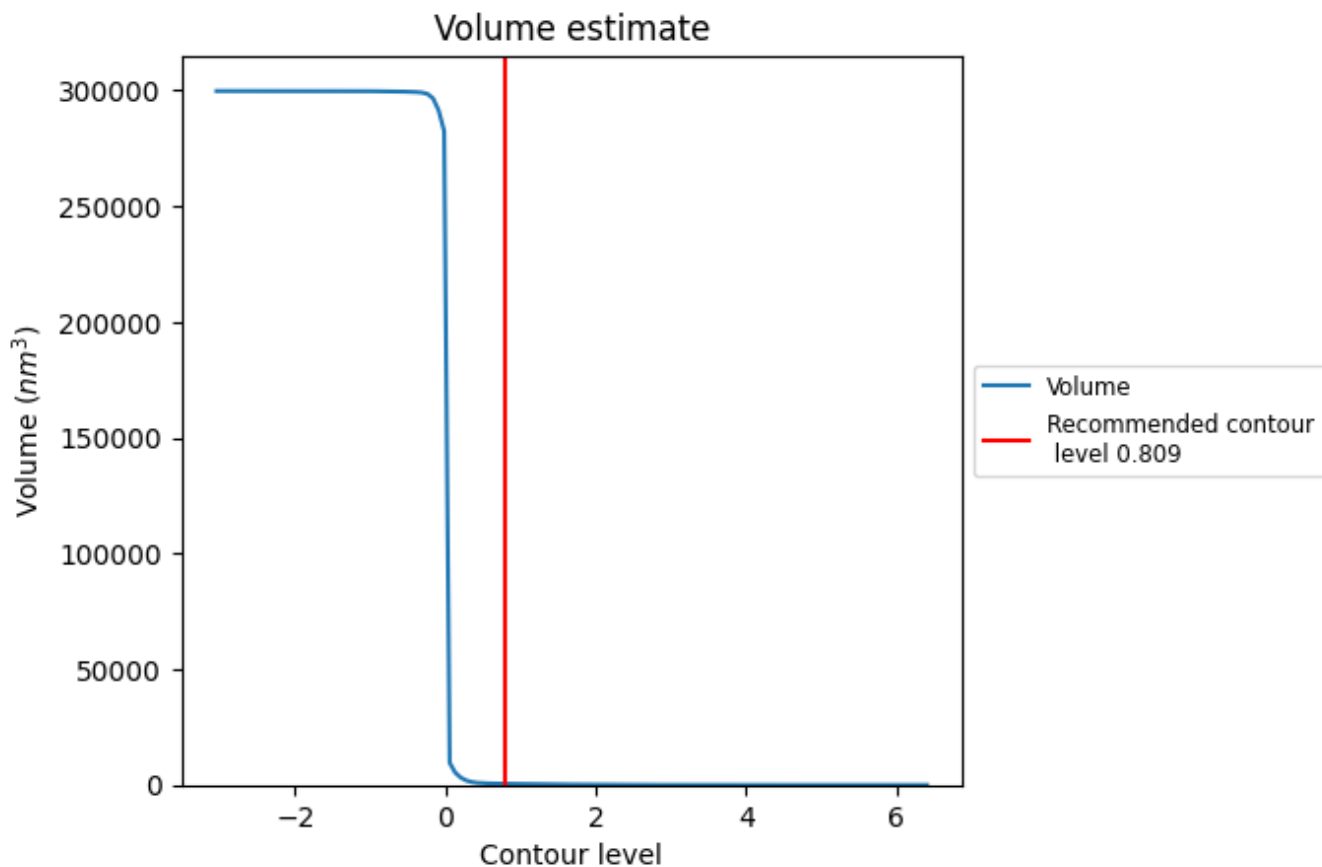
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

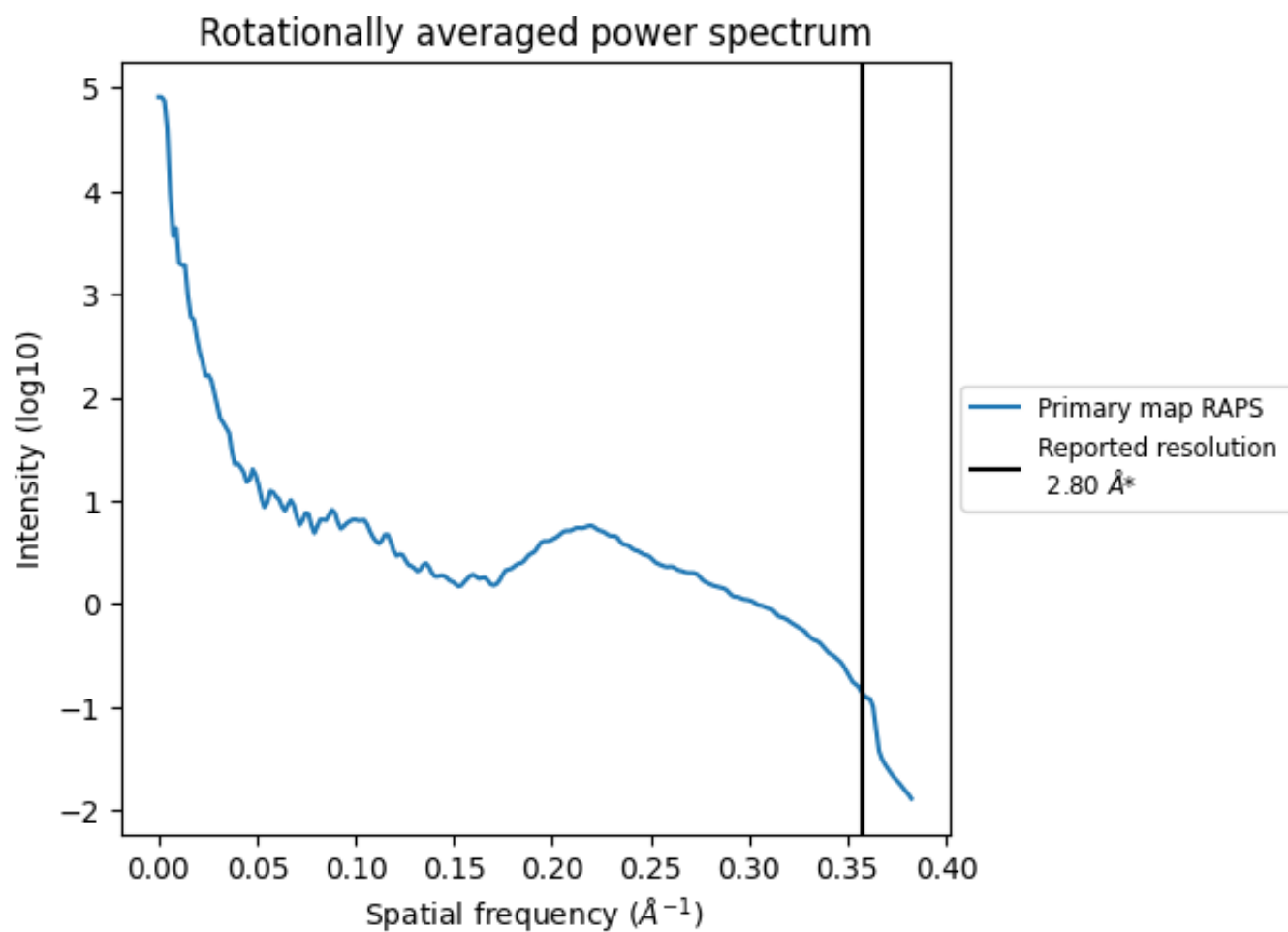
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 503 nm<sup>3</sup>; this corresponds to an approximate mass of 455 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of 0.357 Å<sup>-1</sup>

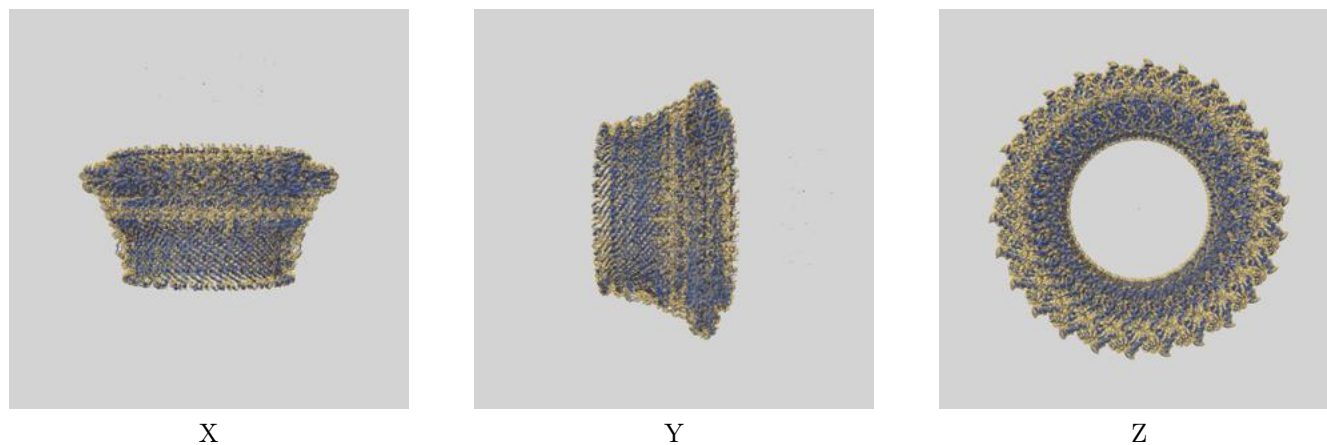
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

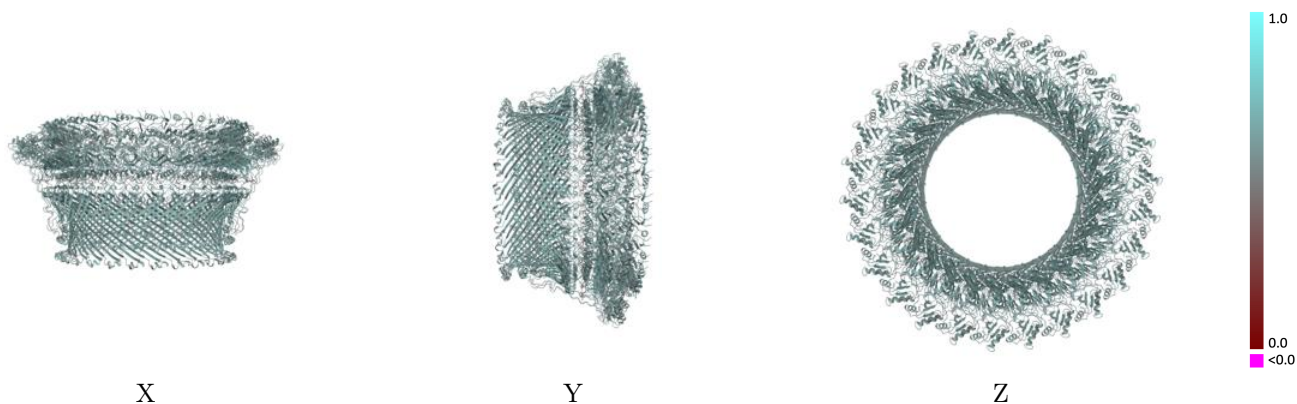
This section contains information regarding the fit between EMDB map EMD-30335 and PDB model 7CBL. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



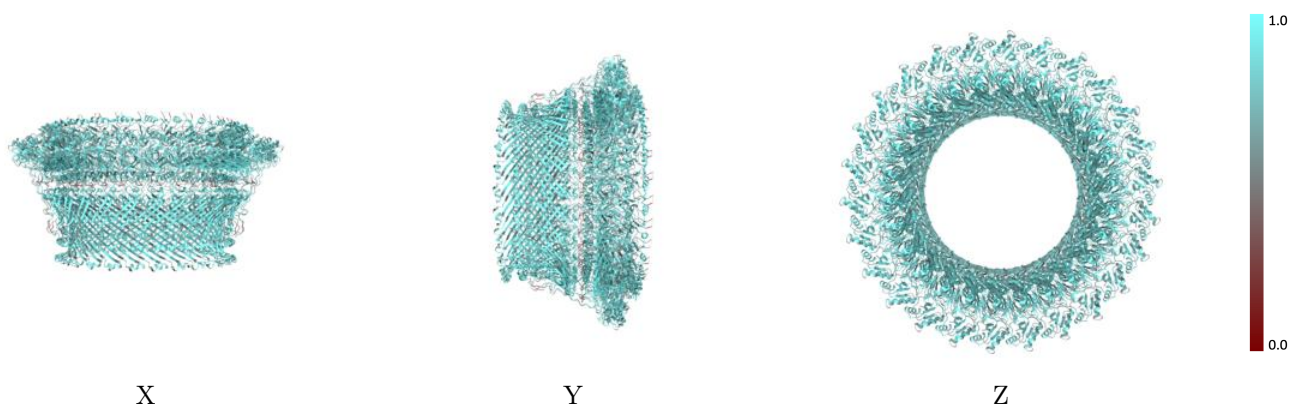
The images above show the 3D surface view of the map at the recommended contour level 0.809 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



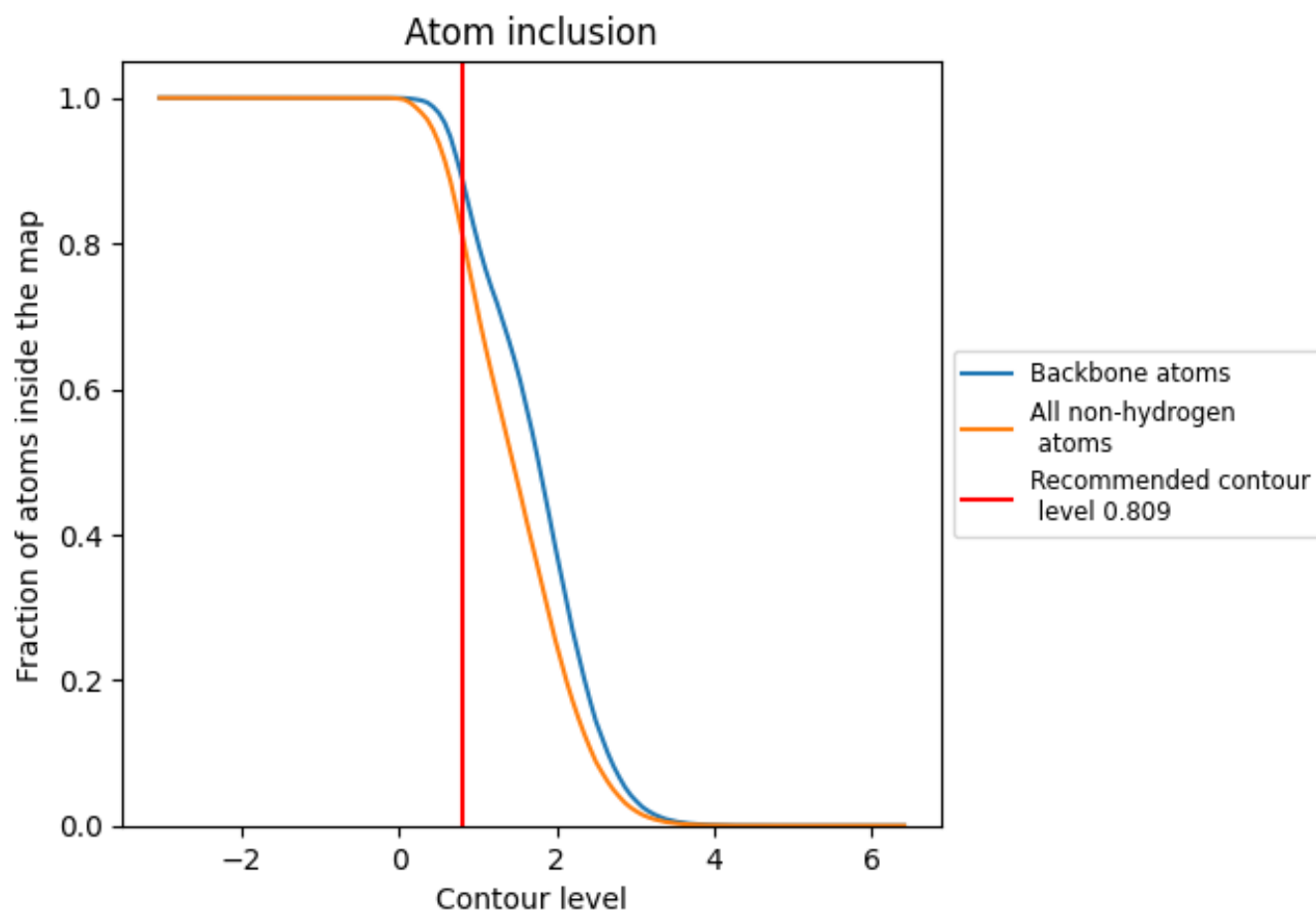
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.809).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.809) and Q-score for the entire model and for each chain.





































Chain	Atom inclusion	Q-score
All	 0.8077	 0.5880
A	 0.7964	 0.5840
B	 0.7996	 0.5880
C	 0.7919	 0.5880
D	 0.7913	 0.5880
E	 0.7971	 0.5890
F	 0.7951	 0.5870
G	 0.7983	 0.5860
H	 0.8105	 0.5910
I	 0.8169	 0.5920
J	 0.8227	 0.5930
K	 0.8227	 0.5890
L	 0.8374	 0.5910
M	 0.8303	 0.5900
N	 0.8201	 0.5910
O	 0.8291	 0.5920
P	 0.8156	 0.5920
Q	 0.8233	 0.5890
R	 0.8150	 0.5900
S	 0.8182	 0.5910
T	 0.8284	 0.5900
U	 0.8259	 0.5910
V	 0.8259	 0.5910
W	 0.8259	 0.5910
X	 0.8239	 0.5900
Y	 0.8099	 0.5930
Z	 0.7990	 0.5900
a	 0.7954	 0.5880
b	 0.7890	 0.5840
c	 0.7808	 0.5840
d	 0.7790	 0.5840
e	 0.7795	 0.5860
f	 0.7900	 0.5860
g	 0.7950	 0.5880
h	 0.7913	 0.5880



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Chain	Atom inclusion	Q-score
i	 0.8096	 0.5870
j	 0.8119	 0.5890
k	 0.8151	 0.5920
l	 0.8160	 0.5930
m	 0.8196	 0.5890
n	 0.8215	 0.5910
o	 0.8091	 0.5910
p	 0.8091	 0.5890
q	 0.8055	 0.5890
r	 0.8009	 0.5820
s	 0.8032	 0.5860
t	 0.8082	 0.5810
u	 0.8114	 0.5820
v	 0.8018	 0.5750
w	 0.8183	 0.5870
x	 0.8224	 0.5890
y	 0.8078	 0.5880
z	 0.7895	 0.5770