



Full wwPDB EM Validation Report ⓘ

Aug 26, 2024 – 02:50 PM EDT

PDB ID : 8CYG
EMDB ID : EMD-27077
Title : Cryo-EM structure of TTMV-LY1 anellovirus virus-like particle
Authors : Liou, S.H.; Delagrave, S.; Swanson, K.
Deposited on : 2022-05-23
Resolution : 3.98 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

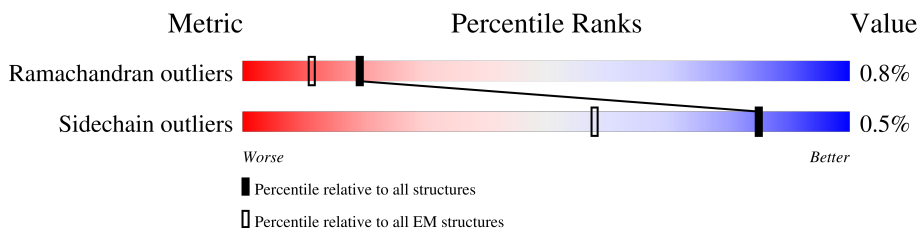
EMDB validation analysis : 0.0.1.dev112
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

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 3.98 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	0	672	8% (red), 71% (green), 27% (grey), 8% (orange)
1	1	672	12% (red), 71% (green), 27% (grey), 8% (orange)
1	2	672	13% (red), 71% (green), 27% (grey), 8% (orange)
1	3	672	8% (red), 71% (green), 27% (grey), 8% (orange)
1	4	672	8% (red), 71% (green), 27% (grey), 8% (orange)
1	5	672	8% (red), 71% (green), 27% (grey), 8% (orange)
1	6	672	7% (red), 71% (green), 27% (grey), 8% (orange)
1	7	672	7% (red), 71% (green), 27% (grey), 8% (orange)
1	A	672	12% (red), 71% (green), 27% (grey), 8% (orange)

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Mol	Chain	Length	Quality of chain		
1	B	672	10%	71%	27%
1	C	672	9%	71%	27%
1	D	672	11%	71%	27%
1	E	672	11%	71%	27%
1	F	672	10%	71%	27%
1	G	672	10%	71%	27%
1	H	672	9%	71%	27%
1	I	672	8%	71%	27%
1	J	672	8%	71%	27%
1	K	672	7%	71%	27%
1	L	672	7%	71%	27%
1	M	672	8%	71%	27%
1	N	672	10%	71%	27%
1	O	672	15%	71%	27%
1	P	672	10%	71%	27%
1	Q	672	9%	71%	27%
1	R	672	10%	71%	27%
1	S	672	10%	71%	27%
1	T	672	12%	71%	27%
1	U	672	10%	71%	27%
1	V	672	13%	71%	27%
1	W	672	11%	71%	27%
1	X	672	9%	71%	27%
1	Y	672	10%	71%	27%
1	Z	672	8%	71%	27%

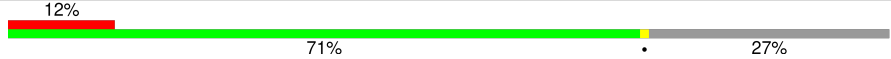
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Mol	Chain	Length	Quality of chain		
1	a	672	8%	71%	27%
1	b	672	8%	71%	27%
1	c	672	7%	71%	27%
1	d	672	7%	71%	27%
1	e	672	8%	71%	27%
1	f	672	7%	71%	27%
1	g	672	8%	71%	27%
1	h	672	7%	71%	27%
1	i	672	8%	71%	27%
1	j	672	8%	71%	27%
1	k	672	8%	71%	27%
1	l	672	8%	71%	27%
1	m	672	8%	71%	27%
1	n	672	8%	71%	27%
1	o	672	8%	71%	27%
1	p	672	8%	71%	27%
1	q	672	8%	71%	27%
1	r	672	8%	71%	27%
1	s	672	7%	71%	27%
1	t	672	10%	71%	27%
1	u	672	8%	71%	27%
1	v	672	7%	71%	27%
1	w	672	8%	71%	27%
1	x	672	8%	71%	27%
1	y	672	8%	71%	27%

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Mol	Chain	Length	Quality of chain
1	z	672	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a green segment in the middle labeled '71%', and a grey segment on the right labeled '27%'. A small black dot is located at the end of the grey segment.</p>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 234597 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	490	3910	2496	664	736	14	0	0
1	a	490	3910	2496	664	736	14	0	0
1	b	490	3910	2496	664	736	14	0	0
1	c	490	3910	2496	664	736	14	0	0
1	d	490	3910	2496	664	736	14	0	0
1	3	490	3910	2496	664	736	14	0	0
1	4	490	3910	2496	664	736	14	0	0
1	5	490	3910	2496	664	736	14	0	0
1	6	490	3910	2496	664	736	14	0	0
1	7	490	3910	2496	664	736	14	0	0
1	I	490	3910	2496	664	736	14	0	0
1	J	490	3910	2496	664	736	14	0	0
1	K	490	3910	2496	664	736	14	0	0
1	L	490	3910	2496	664	736	14	0	0
1	M	490	3910	2496	664	736	14	0	0
1	e	490	3910	2496	664	736	14	0	0
1	f	490	3910	2496	664	736	14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	h	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	i	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	j	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	k	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	l	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	m	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	n	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	o	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	p	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	q	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	r	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	s	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	t	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	u	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	v	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	w	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	x	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	y	490	Total	C	N	O	S	0	0
			3909	2495	664	736	14		
1	1	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		
1	2	490	Total	C	N	O	S	0	0
			3910	2496	664	736	14		

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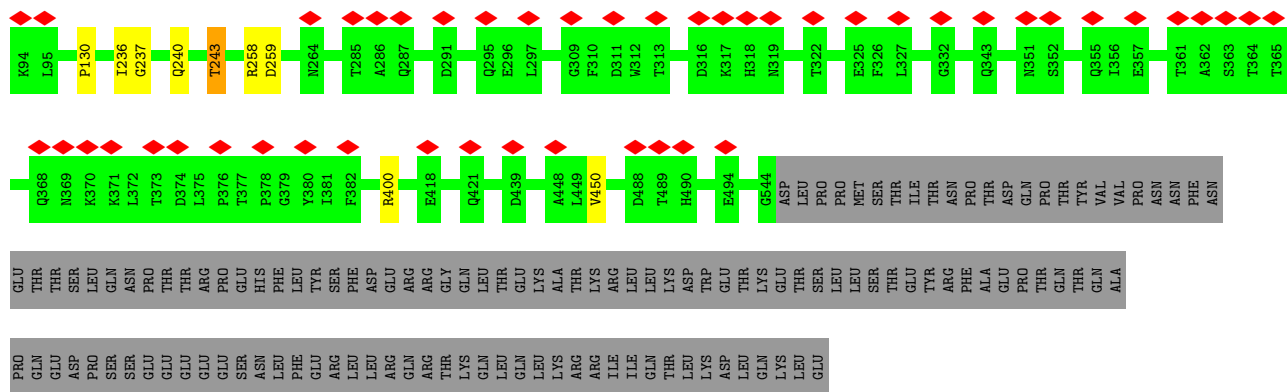
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	z	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	A	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	B	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	D	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	E	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	F	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	G	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	H	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	N	490	Total 3909	C 2495	N 664	O 736	S 14	0	0
1	P	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	Q	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	R	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	T	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	U	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	V	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	W	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	X	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	Y	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	Z	490	Total 3910	C 2496	N 664	O 736	S 14	0	0
1	C	490	Total 3910	C 2496	N 664	O 736	S 14	0	0

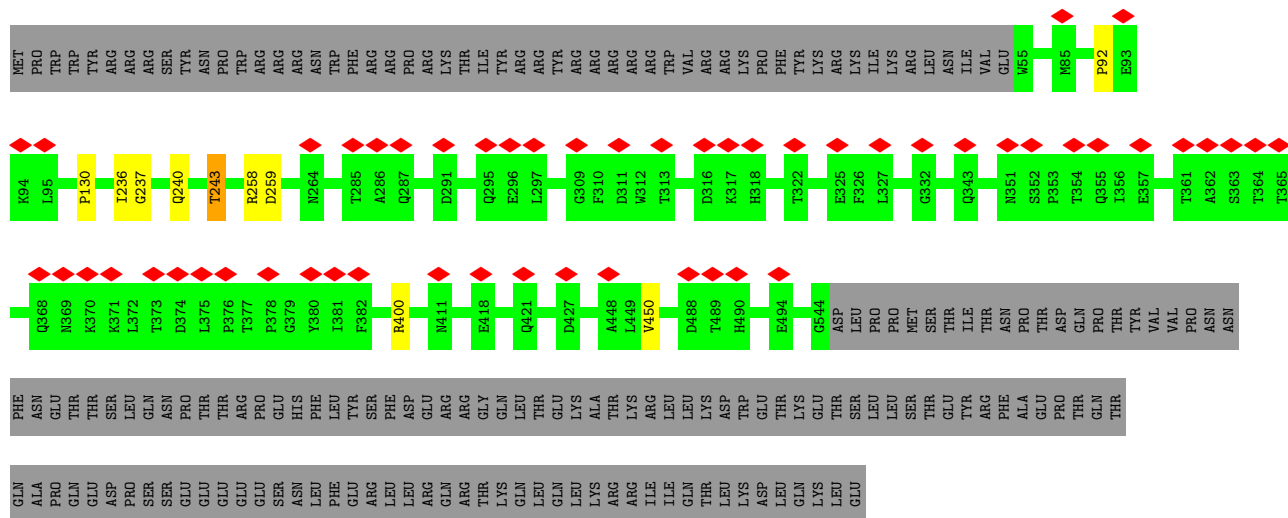
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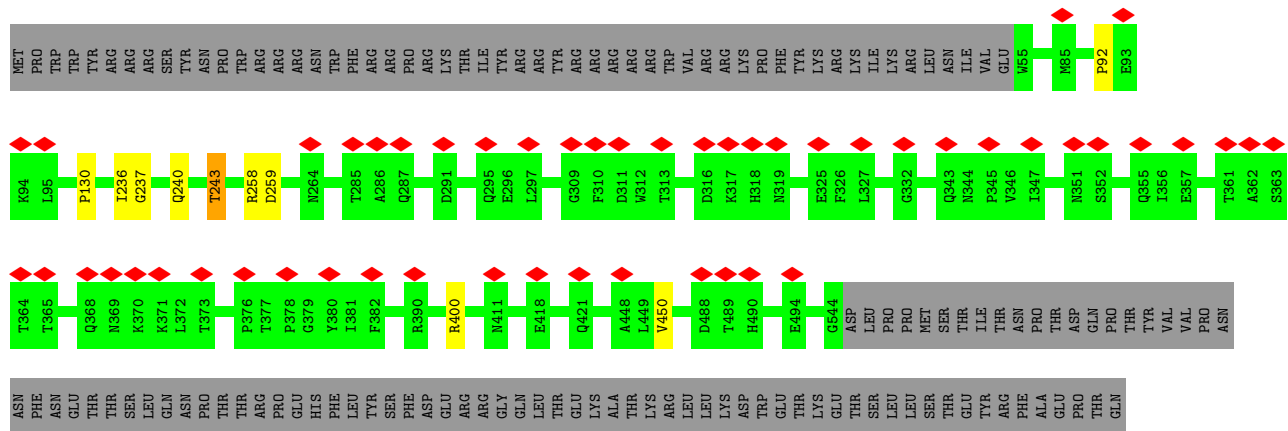
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	S	490	3909	2495	664	736	14	0	0

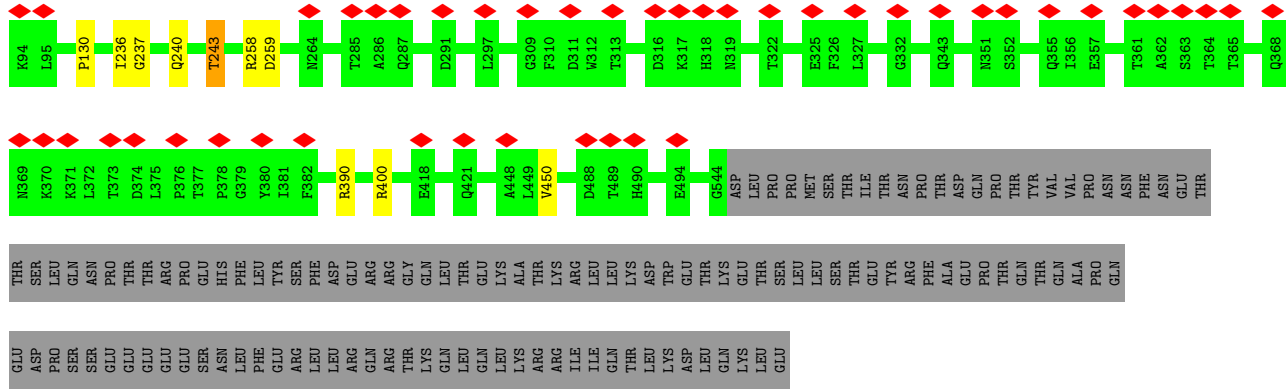


• Molecule 1: Capsid protein

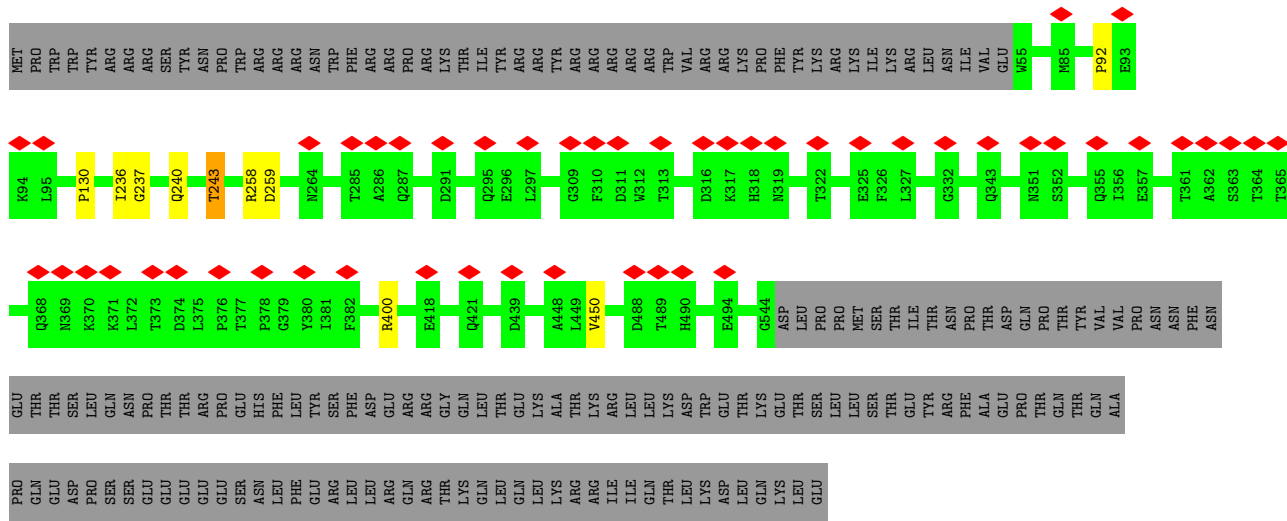


• Molecule 1: Capsid protein

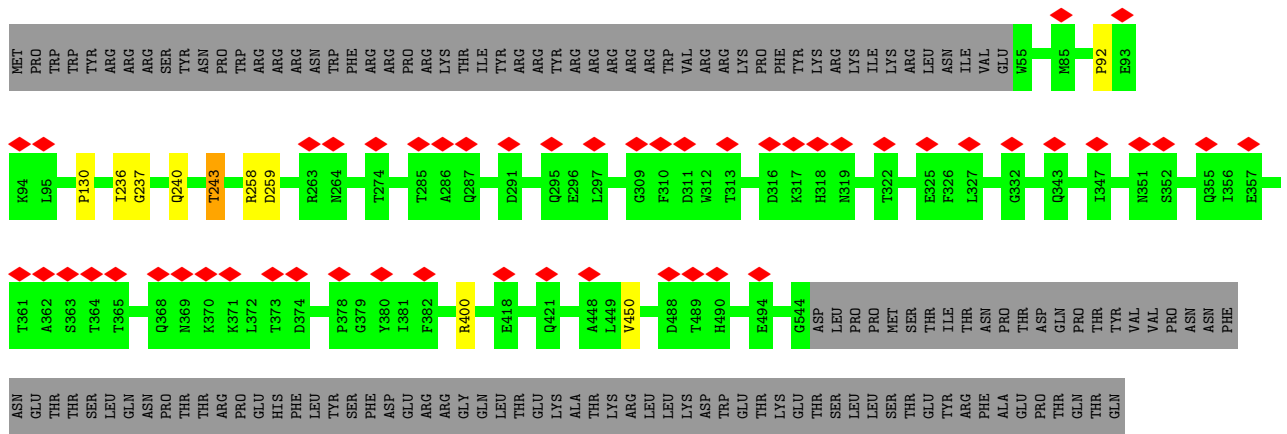


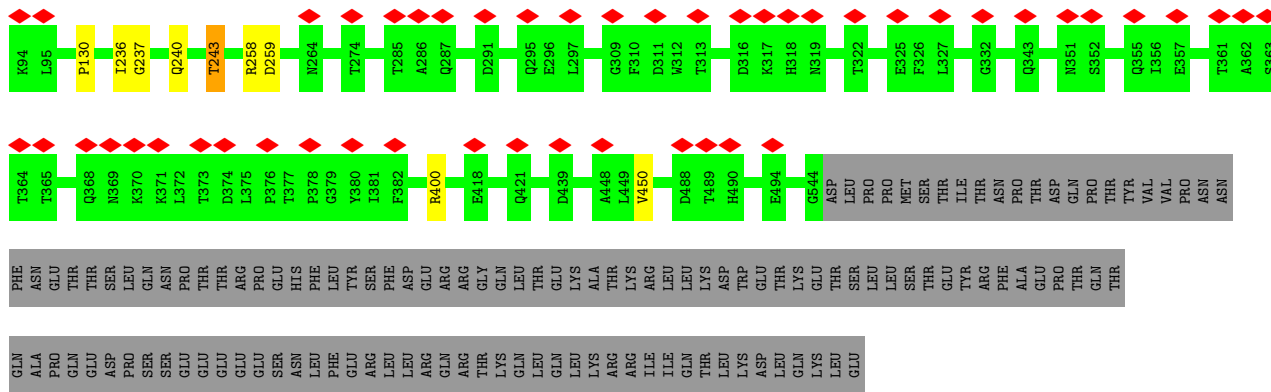


● Molecule 1: Capsid protein

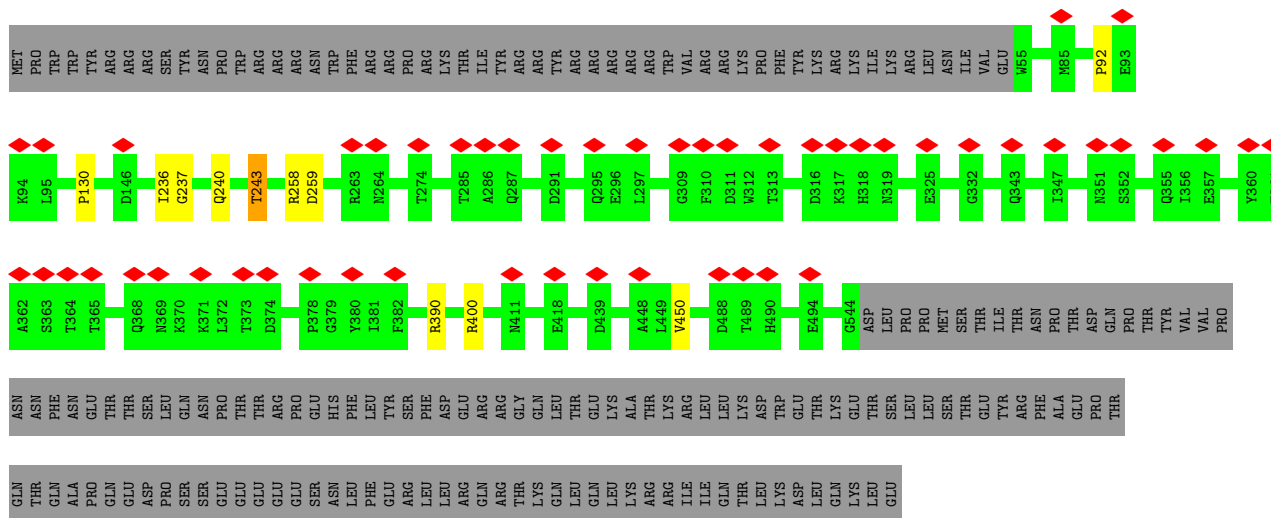


● Molecule 1: Capsid protein

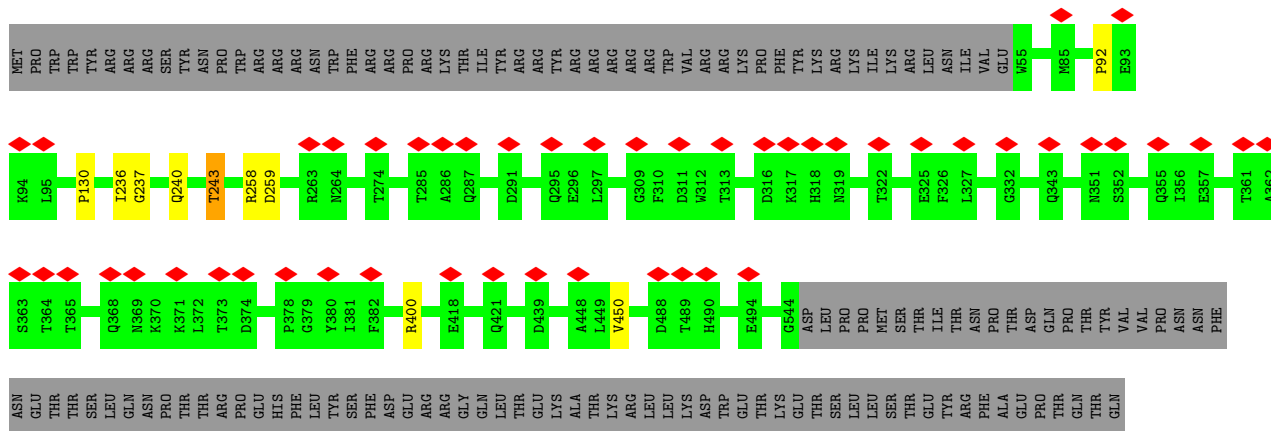


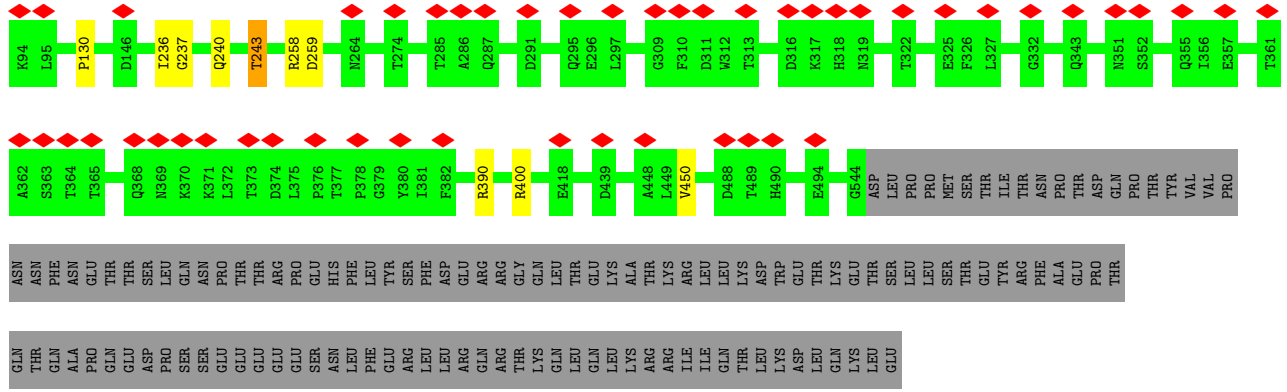


• Molecule 1: Capsid protein

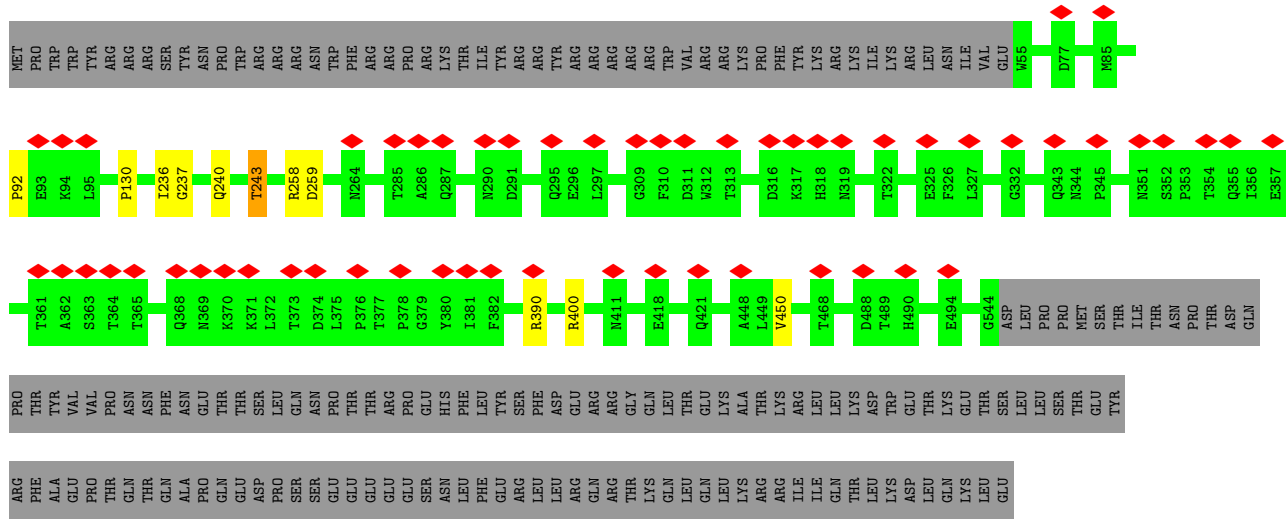


• Molecule 1: Capsid protein

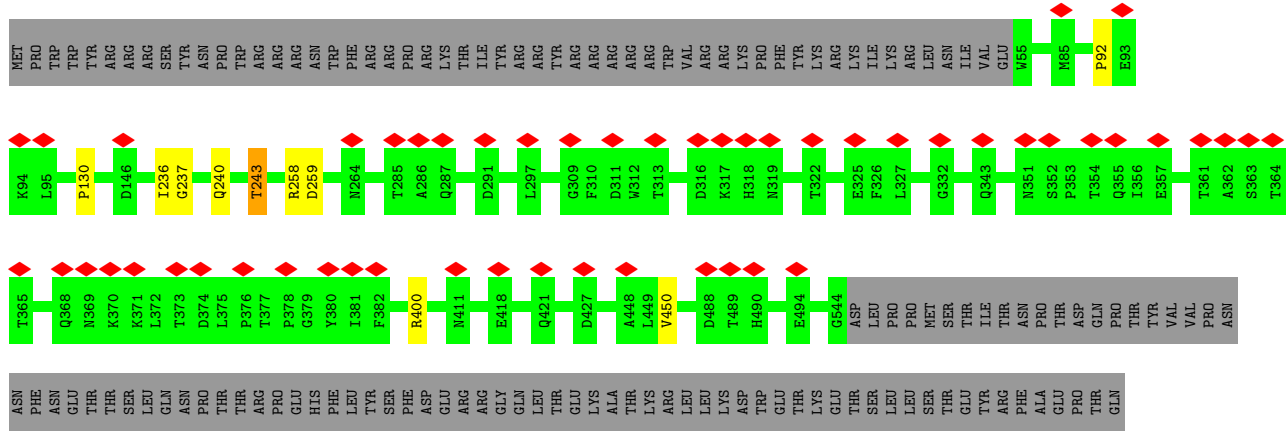
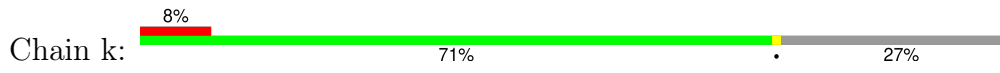




• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



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• Molecule 1: Capsid protein



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• Molecule 1: Capsid protein



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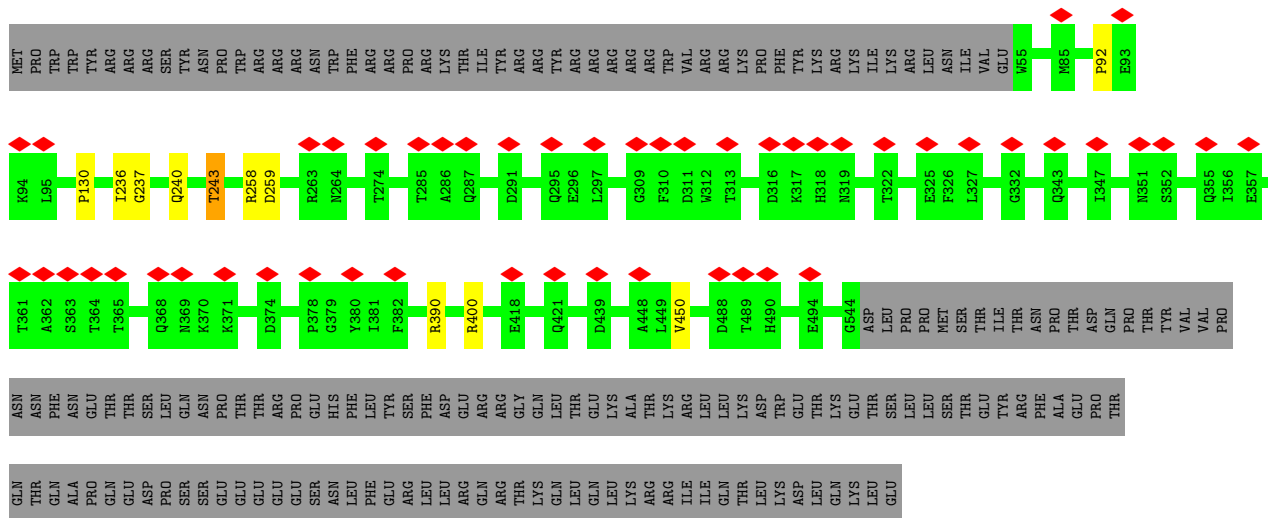
• Molecule 1: Capsid protein



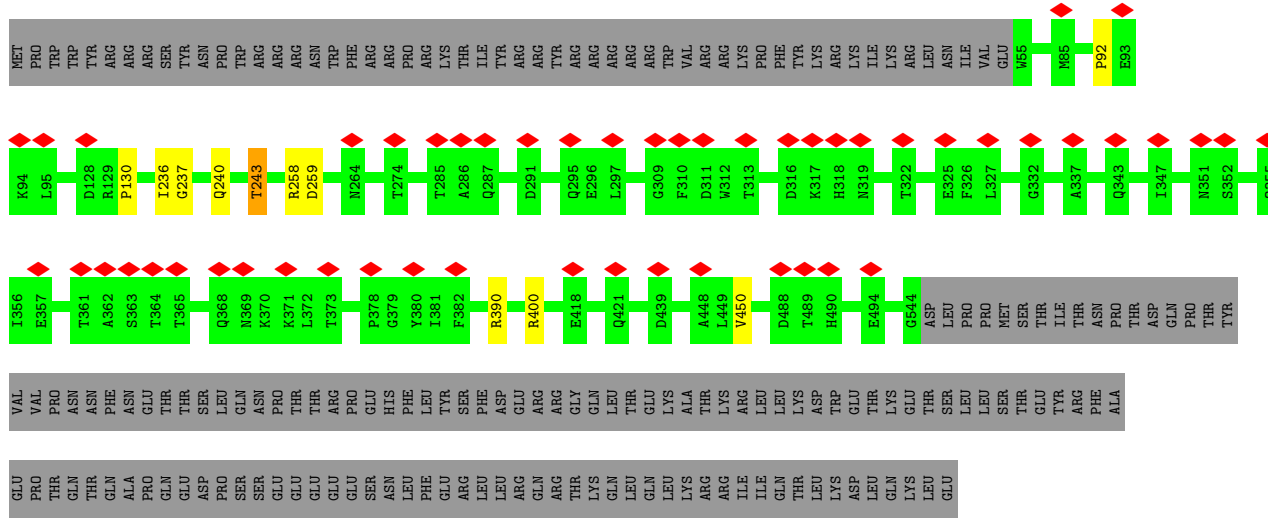
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• Molecule 1: Capsid protein

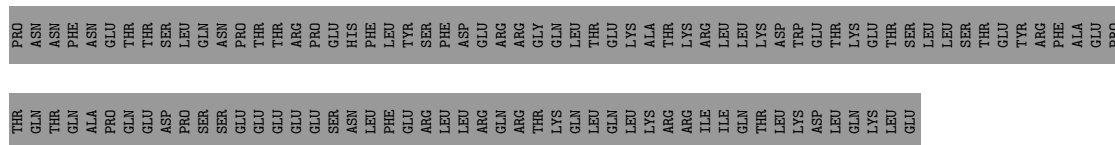


• Molecule 1: Capsid protein

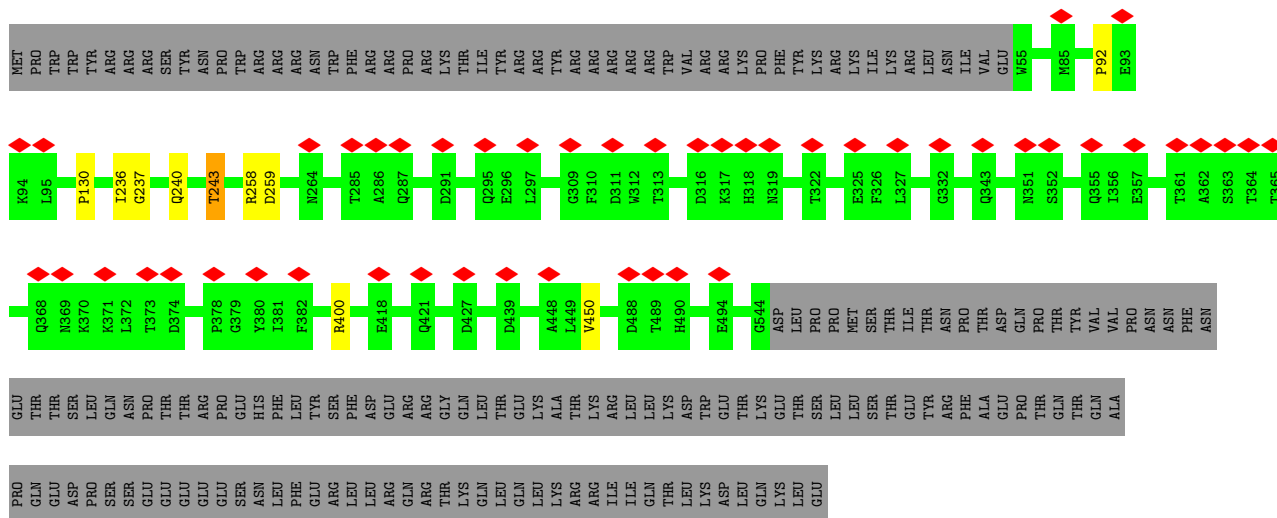


• Molecule 1: Capsid protein

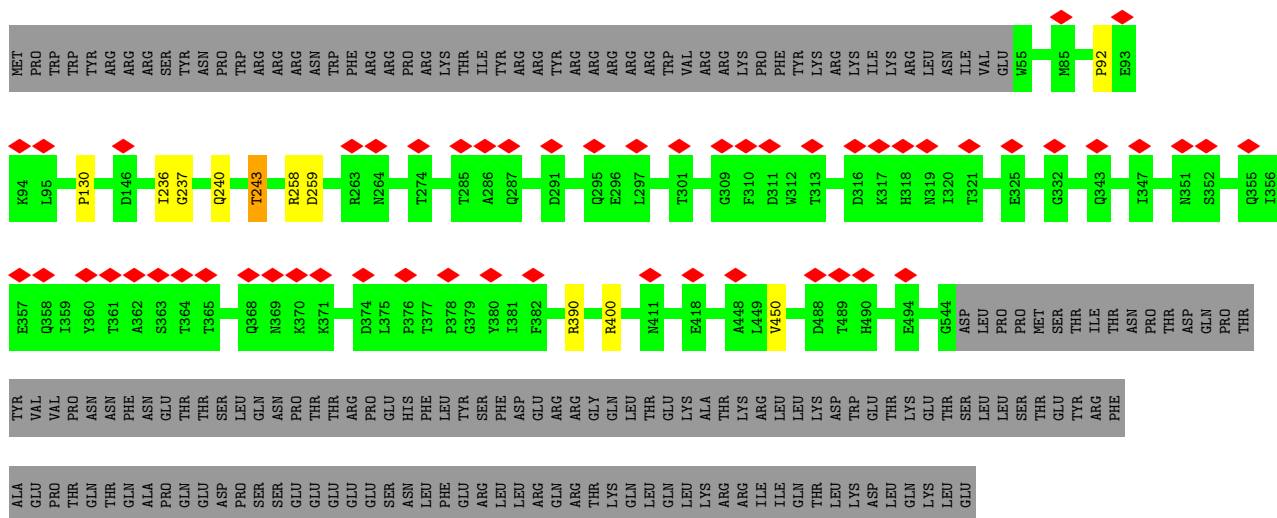




• Molecule 1: Capsid protein

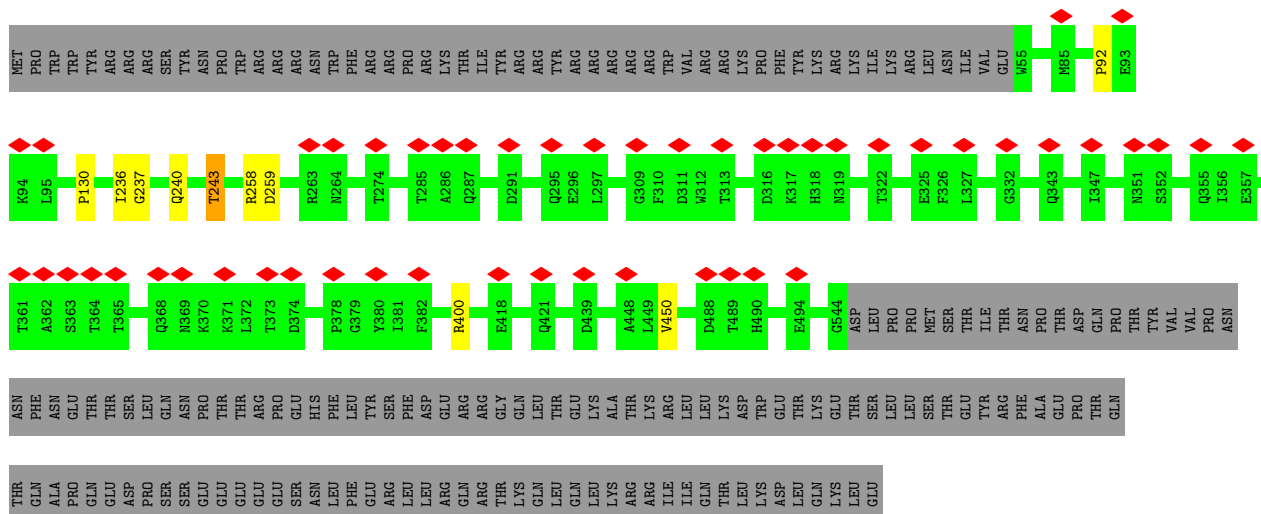


• Molecule 1: Capsid protein

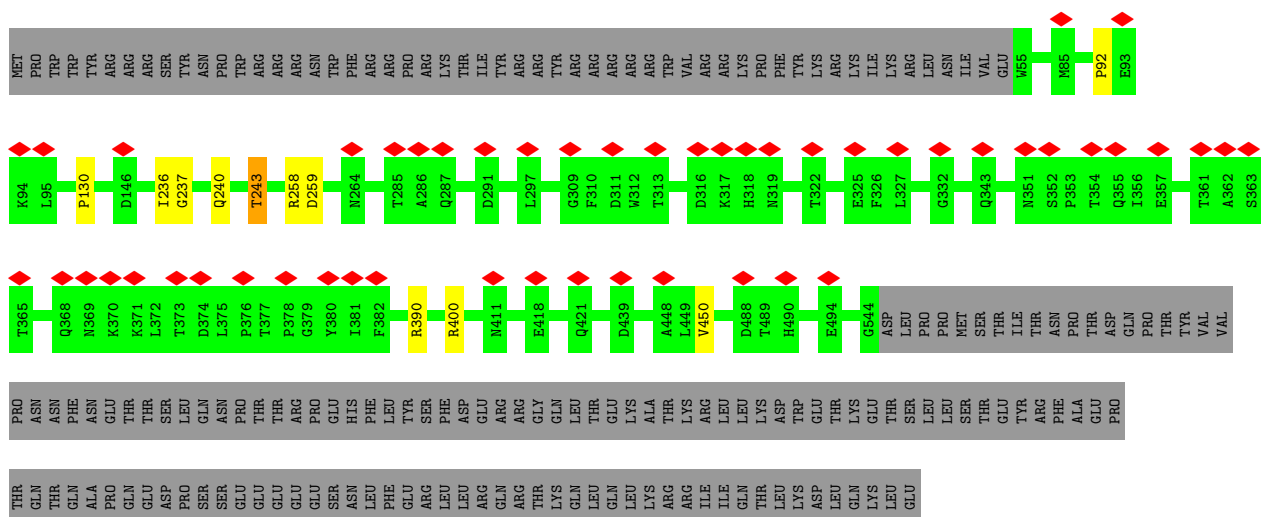


• Molecule 1: Capsid protein

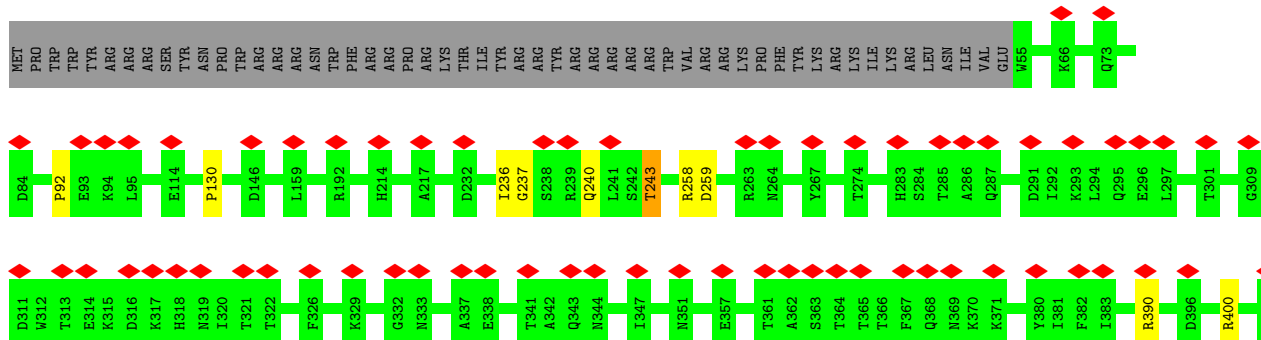


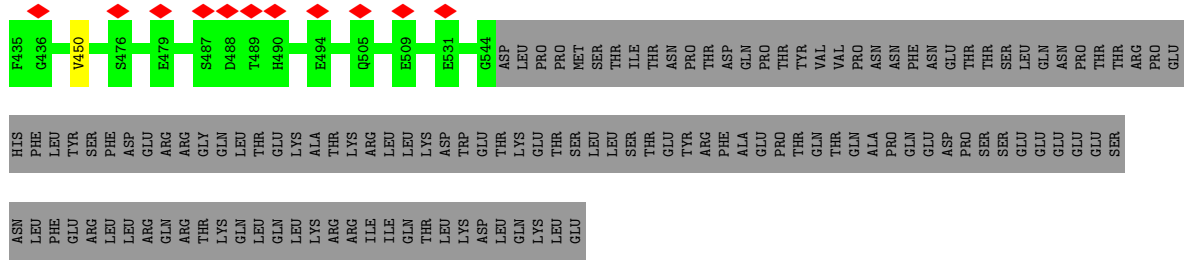


• Molecule 1: Capsid protein

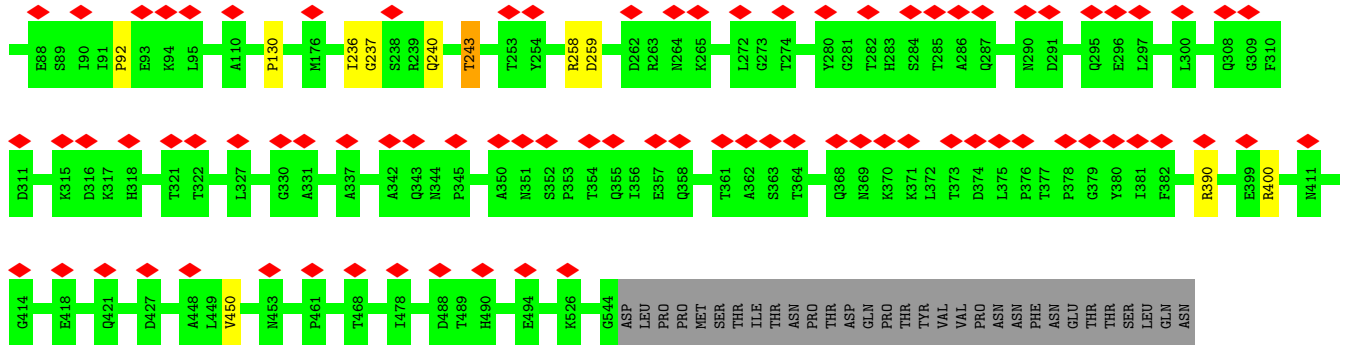


• Molecule 1: Capsid protein

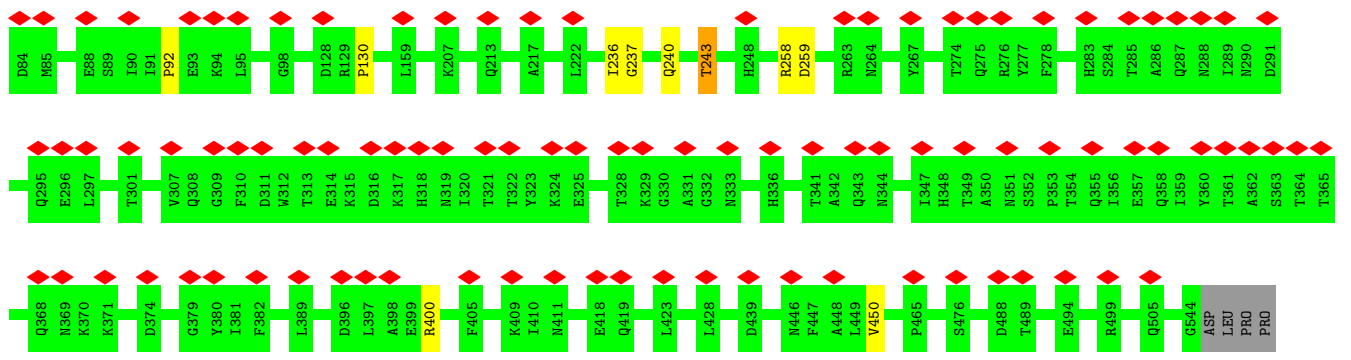


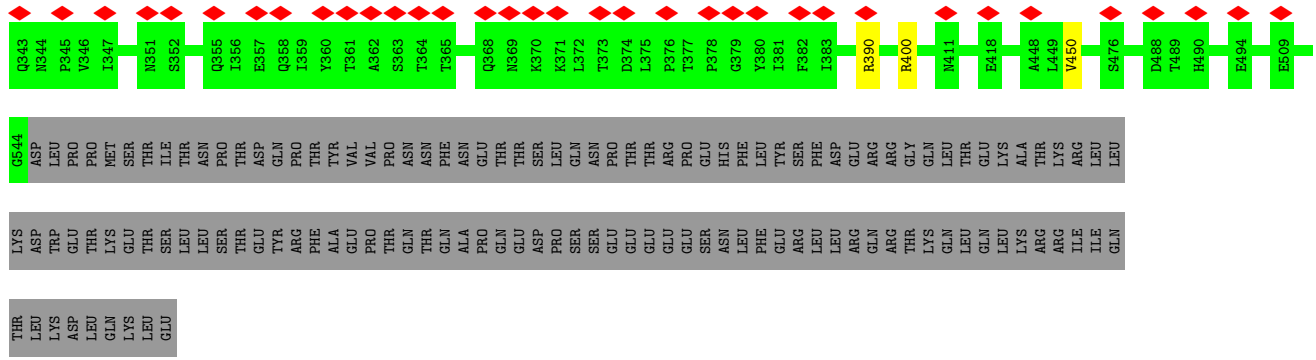


• Molecule 1: Capsid protein

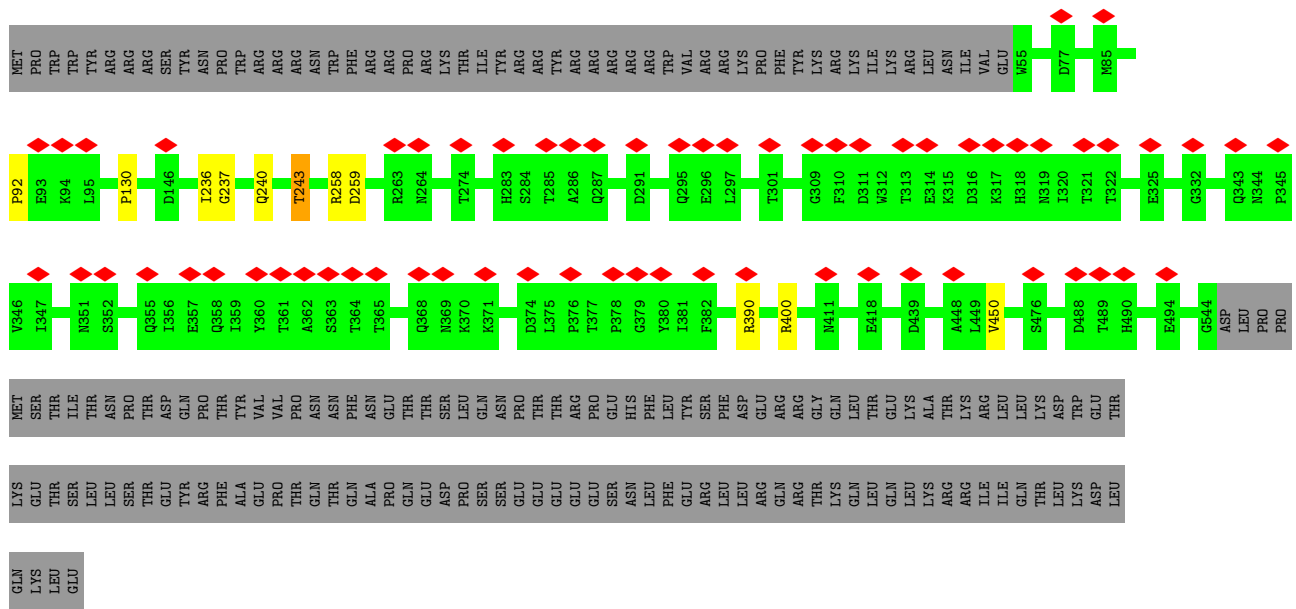


• Molecule 1: Capsid protein

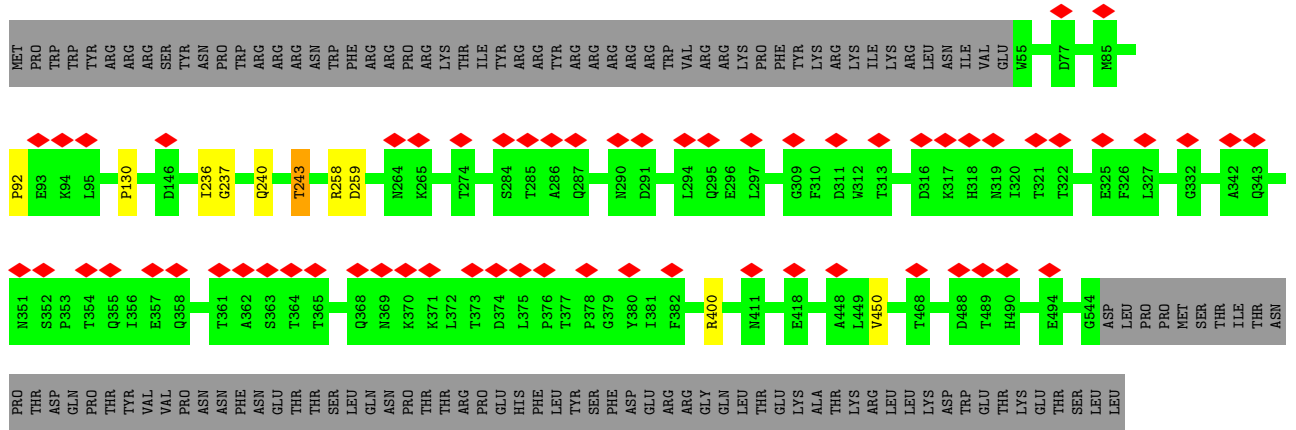




• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6271	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	19.59	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	14.536	Depositor
Minimum map value	-10.424	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.87	Depositor
Map size (Å)	406.12, 406.12, 406.12	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.923, 0.923, 0.923	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	1	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	2	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	3	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	4	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	5	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	6	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	7	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	A	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	B	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	C	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	D	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	E	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	F	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	G	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	H	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	I	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	J	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	K	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	L	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	M	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	N	0.45	1/4018 (0.0%)	0.77	7/5476 (0.1%)
1	O	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	P	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	Q	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	R	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	S	0.45	1/4018 (0.0%)	0.77	6/5476 (0.1%)
1	T	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	U	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	V	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	W	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	X	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	Y	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	Z	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	b	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	c	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	d	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	e	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	f	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	g	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	h	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	i	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	j	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	k	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	l	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	m	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	n	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	o	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	p	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	q	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	r	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	s	0.45	1/4020 (0.0%)	0.77	7/5480 (0.1%)
1	t	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	u	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	v	0.45	1/4020 (0.0%)	0.76	6/5480 (0.1%)
1	w	0.45	1/4020 (0.0%)	0.76	7/5480 (0.1%)
1	x	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
1	y	0.45	1/4018 (0.0%)	0.77	7/5476 (0.1%)
1	z	0.45	1/4020 (0.0%)	0.77	6/5480 (0.1%)
All	All	0.45	60/241194 (0.0%)	0.77	388/328788 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
1	1	0	2
1	2	0	2
1	3	0	2
1	4	0	2
1	5	0	2
1	6	0	2
1	7	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
1	a	0	2
1	b	0	2
1	c	0	2
1	d	0	2
1	e	0	2
1	f	0	2
1	g	0	2
1	h	0	2
1	i	0	2
1	j	0	2
1	k	0	2
1	l	0	2
1	m	0	2
1	n	0	2
1	o	0	2
1	p	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	2
1	r	0	2
1	s	0	2
1	t	0	2
1	u	0	2
1	v	0	2
1	w	0	2
1	x	0	2
1	y	0	2
1	z	0	2
All	All	0	120

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	243	THR	C-N	-11.17	1.08	1.34
1	F	243	THR	C-N	-11.16	1.08	1.34
1	P	243	THR	C-N	-11.16	1.08	1.34
1	5	243	THR	C-N	-11.16	1.08	1.34
1	E	243	THR	C-N	-11.15	1.08	1.34
1	D	243	THR	C-N	-11.15	1.08	1.34
1	y	243	THR	C-N	-11.15	1.08	1.34
1	2	243	THR	C-N	-11.15	1.08	1.34
1	L	243	THR	C-N	-11.14	1.08	1.34
1	A	243	THR	C-N	-11.14	1.08	1.34
1	h	243	THR	C-N	-11.14	1.08	1.34
1	z	243	THR	C-N	-11.14	1.08	1.34
1	i	243	THR	C-N	-11.14	1.08	1.34
1	w	243	THR	C-N	-11.14	1.08	1.34
1	S	243	THR	C-N	-11.14	1.08	1.34
1	t	243	THR	C-N	-11.14	1.08	1.34
1	7	243	THR	C-N	-11.13	1.08	1.34
1	d	243	THR	C-N	-11.13	1.08	1.34
1	r	243	THR	C-N	-11.13	1.08	1.34
1	Q	243	THR	C-N	-11.13	1.08	1.34
1	b	243	THR	C-N	-11.12	1.08	1.34
1	v	243	THR	C-N	-11.13	1.08	1.34
1	c	243	THR	C-N	-11.12	1.08	1.34
1	4	243	THR	C-N	-11.12	1.08	1.34
1	k	243	THR	C-N	-11.12	1.08	1.34
1	V	243	THR	C-N	-11.12	1.08	1.34
1	W	243	THR	C-N	-11.12	1.08	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	m	243	THR	C-N	-11.12	1.08	1.34
1	n	243	THR	C-N	-11.12	1.08	1.34
1	s	243	THR	C-N	-11.12	1.08	1.34
1	I	243	THR	C-N	-11.12	1.08	1.34
1	o	243	THR	C-N	-11.11	1.08	1.34
1	O	243	THR	C-N	-11.11	1.08	1.34
1	B	243	THR	C-N	-11.11	1.08	1.34
1	C	243	THR	C-N	-11.11	1.08	1.34
1	0	243	THR	C-N	-11.11	1.08	1.34
1	6	243	THR	C-N	-11.11	1.08	1.34
1	J	243	THR	C-N	-11.11	1.08	1.34
1	g	243	THR	C-N	-11.11	1.08	1.34
1	a	243	THR	C-N	-11.10	1.08	1.34
1	e	243	THR	C-N	-11.10	1.08	1.34
1	l	243	THR	C-N	-11.10	1.08	1.34
1	q	243	THR	C-N	-11.10	1.08	1.34
1	N	243	THR	C-N	-11.10	1.08	1.34
1	Z	243	THR	C-N	-11.10	1.08	1.34
1	K	243	THR	C-N	-11.10	1.08	1.34
1	R	243	THR	C-N	-11.10	1.08	1.34
1	T	243	THR	C-N	-11.10	1.08	1.34
1	U	243	THR	C-N	-11.10	1.08	1.34
1	G	243	THR	C-N	-11.10	1.08	1.34
1	1	243	THR	C-N	-11.09	1.08	1.34
1	j	243	THR	C-N	-11.09	1.08	1.34
1	3	243	THR	C-N	-11.08	1.08	1.34
1	f	243	THR	C-N	-11.08	1.08	1.34
1	H	243	THR	C-N	-11.08	1.08	1.34
1	X	243	THR	C-N	-11.07	1.08	1.34
1	x	243	THR	C-N	-11.07	1.08	1.34
1	Y	243	THR	C-N	-11.07	1.08	1.34
1	p	243	THR	C-N	-11.07	1.08	1.34
1	u	243	THR	C-N	-11.06	1.08	1.34

All (388) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	243	THR	O-C-N	-21.27	88.67	122.70
1	V	243	THR	O-C-N	-21.27	88.67	122.70
1	H	243	THR	O-C-N	-21.27	88.67	122.70
1	3	243	THR	O-C-N	-21.26	88.68	122.70
1	f	243	THR	O-C-N	-21.26	88.68	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	243	THR	O-C-N	-21.26	88.68	122.70
1	n	243	THR	O-C-N	-21.26	88.68	122.70
1	6	243	THR	O-C-N	-21.25	88.70	122.70
1	h	243	THR	O-C-N	-21.25	88.70	122.70
1	W	243	THR	O-C-N	-21.25	88.70	122.70
1	p	243	THR	O-C-N	-21.25	88.71	122.70
1	s	243	THR	O-C-N	-21.25	88.71	122.70
1	2	243	THR	O-C-N	-21.25	88.71	122.70
1	B	243	THR	O-C-N	-21.25	88.71	122.70
1	y	243	THR	O-C-N	-21.24	88.71	122.70
1	C	243	THR	O-C-N	-21.24	88.71	122.70
1	c	243	THR	O-C-N	-21.24	88.72	122.70
1	7	243	THR	O-C-N	-21.24	88.72	122.70
1	l	243	THR	O-C-N	-21.24	88.72	122.70
1	P	243	THR	O-C-N	-21.24	88.72	122.70
1	Y	243	THR	O-C-N	-21.24	88.72	122.70
1	J	243	THR	O-C-N	-21.24	88.72	122.70
1	r	243	THR	O-C-N	-21.24	88.72	122.70
1	a	243	THR	O-C-N	-21.23	88.72	122.70
1	j	243	THR	O-C-N	-21.23	88.73	122.70
1	F	243	THR	O-C-N	-21.23	88.73	122.70
1	S	243	THR	O-C-N	-21.23	88.73	122.70
1	e	243	THR	O-C-N	-21.23	88.74	122.70
1	t	243	THR	O-C-N	-21.23	88.74	122.70
1	G	243	THR	O-C-N	-21.23	88.74	122.70
1	0	243	THR	O-C-N	-21.23	88.74	122.70
1	A	243	THR	O-C-N	-21.23	88.74	122.70
1	d	243	THR	O-C-N	-21.22	88.74	122.70
1	k	243	THR	O-C-N	-21.22	88.74	122.70
1	u	243	THR	O-C-N	-21.22	88.74	122.70
1	4	243	THR	O-C-N	-21.22	88.75	122.70
1	L	243	THR	O-C-N	-21.22	88.74	122.70
1	I	243	THR	O-C-N	-21.22	88.75	122.70
1	v	243	THR	O-C-N	-21.22	88.75	122.70
1	U	243	THR	O-C-N	-21.22	88.75	122.70
1	K	243	THR	O-C-N	-21.22	88.75	122.70
1	X	243	THR	O-C-N	-21.22	88.75	122.70
1	1	243	THR	O-C-N	-21.21	88.76	122.70
1	R	243	THR	O-C-N	-21.21	88.76	122.70
1	T	243	THR	O-C-N	-21.21	88.76	122.70
1	O	243	THR	O-C-N	-21.21	88.76	122.70
1	o	243	THR	O-C-N	-21.21	88.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	243	THR	O-C-N	-21.21	88.77	122.70
1	z	243	THR	O-C-N	-21.20	88.77	122.70
1	M	243	THR	O-C-N	-21.20	88.78	122.70
1	b	243	THR	O-C-N	-21.20	88.78	122.70
1	i	243	THR	O-C-N	-21.19	88.79	122.70
1	q	243	THR	O-C-N	-21.19	88.79	122.70
1	D	243	THR	O-C-N	-21.19	88.80	122.70
1	N	243	THR	O-C-N	-21.19	88.80	122.70
1	g	243	THR	O-C-N	-21.18	88.81	122.70
1	Q	243	THR	O-C-N	-21.18	88.82	122.70
1	5	243	THR	O-C-N	-21.16	88.84	122.70
1	w	243	THR	O-C-N	-21.15	88.85	122.70
1	Z	243	THR	O-C-N	-21.15	88.85	122.70
1	F	243	THR	CA-C-N	13.91	147.81	117.20
1	7	243	THR	CA-C-N	13.90	147.79	117.20
1	y	243	THR	CA-C-N	13.90	147.79	117.20
1	V	243	THR	CA-C-N	13.90	147.77	117.20
1	h	243	THR	CA-C-N	13.89	147.76	117.20
1	n	243	THR	CA-C-N	13.89	147.76	117.20
1	l	243	THR	CA-C-N	13.89	147.76	117.20
1	o	243	THR	CA-C-N	13.89	147.76	117.20
1	P	243	THR	CA-C-N	13.89	147.76	117.20
1	L	243	THR	CA-C-N	13.89	147.75	117.20
1	t	243	THR	CA-C-N	13.89	147.75	117.20
1	x	243	THR	CA-C-N	13.89	147.75	117.20
1	B	243	THR	CA-C-N	13.89	147.75	117.20
1	W	243	THR	CA-C-N	13.89	147.75	117.20
1	6	243	THR	CA-C-N	13.88	147.75	117.20
1	k	243	THR	CA-C-N	13.88	147.75	117.20
1	c	243	THR	CA-C-N	13.88	147.74	117.20
1	4	243	THR	CA-C-N	13.88	147.74	117.20
1	i	243	THR	CA-C-N	13.88	147.74	117.20
1	m	243	THR	CA-C-N	13.88	147.74	117.20
1	U	243	THR	CA-C-N	13.88	147.74	117.20
1	v	243	THR	CA-C-N	13.88	147.73	117.20
1	2	243	THR	CA-C-N	13.88	147.73	117.20
1	z	243	THR	CA-C-N	13.88	147.73	117.20
1	G	243	THR	CA-C-N	13.88	147.73	117.20
1	E	243	THR	CA-C-N	13.87	147.72	117.20
1	T	243	THR	CA-C-N	13.87	147.72	117.20
1	0	243	THR	CA-C-N	13.87	147.72	117.20
1	a	243	THR	CA-C-N	13.87	147.72	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	243	THR	CA-C-N	13.87	147.72	117.20
1	3	243	THR	CA-C-N	13.87	147.72	117.20
1	e	243	THR	CA-C-N	13.87	147.72	117.20
1	j	243	THR	CA-C-N	13.87	147.72	117.20
1	q	243	THR	CA-C-N	13.87	147.72	117.20
1	R	243	THR	CA-C-N	13.87	147.72	117.20
1	r	243	THR	CA-C-N	13.87	147.72	117.20
1	p	243	THR	CA-C-N	13.87	147.72	117.20
1	s	243	THR	CA-C-N	13.87	147.71	117.20
1	5	243	THR	CA-C-N	13.87	147.70	117.20
1	b	243	THR	CA-C-N	13.86	147.70	117.20
1	D	243	THR	CA-C-N	13.86	147.70	117.20
1	Q	243	THR	CA-C-N	13.86	147.70	117.20
1	X	243	THR	CA-C-N	13.86	147.70	117.20
1	C	243	THR	CA-C-N	13.86	147.70	117.20
1	S	243	THR	CA-C-N	13.86	147.70	117.20
1	u	243	THR	CA-C-N	13.86	147.69	117.20
1	A	243	THR	CA-C-N	13.86	147.69	117.20
1	H	243	THR	CA-C-N	13.86	147.69	117.20
1	M	243	THR	CA-C-N	13.86	147.68	117.20
1	f	243	THR	CA-C-N	13.86	147.69	117.20
1	Y	243	THR	CA-C-N	13.86	147.68	117.20
1	J	243	THR	CA-C-N	13.85	147.68	117.20
1	g	243	THR	CA-C-N	13.85	147.68	117.20
1	w	243	THR	CA-C-N	13.85	147.67	117.20
1	N	243	THR	CA-C-N	13.85	147.66	117.20
1	I	243	THR	CA-C-N	13.84	147.65	117.20
1	K	243	THR	CA-C-N	13.84	147.66	117.20
1	Z	243	THR	CA-C-N	13.84	147.65	117.20
1	l	243	THR	CA-C-N	13.84	147.64	117.20
1	O	243	THR	CA-C-N	13.83	147.63	117.20
1	P	243	THR	C-N-CA	12.64	153.30	121.70
1	V	243	THR	C-N-CA	12.63	153.28	121.70
1	h	243	THR	C-N-CA	12.63	153.27	121.70
1	F	243	THR	C-N-CA	12.63	153.27	121.70
1	m	243	THR	C-N-CA	12.62	153.25	121.70
1	s	243	THR	C-N-CA	12.62	153.25	121.70
1	L	243	THR	C-N-CA	12.62	153.24	121.70
1	X	243	THR	C-N-CA	12.62	153.24	121.70
1	o	243	THR	C-N-CA	12.62	153.24	121.70
1	d	243	THR	C-N-CA	12.61	153.24	121.70
1	Q	243	THR	C-N-CA	12.62	153.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	243	THR	C-N-CA	12.61	153.24	121.70
1	r	243	THR	C-N-CA	12.61	153.23	121.70
1	n	243	THR	C-N-CA	12.61	153.23	121.70
1	q	243	THR	C-N-CA	12.61	153.23	121.70
1	E	243	THR	C-N-CA	12.61	153.23	121.70
1	i	243	THR	C-N-CA	12.61	153.23	121.70
1	z	243	THR	C-N-CA	12.61	153.22	121.70
1	W	243	THR	C-N-CA	12.61	153.22	121.70
1	c	243	THR	C-N-CA	12.61	153.22	121.70
1	0	243	THR	C-N-CA	12.60	153.21	121.70
1	A	243	THR	C-N-CA	12.60	153.21	121.70
1	M	243	THR	C-N-CA	12.60	153.20	121.70
1	D	243	THR	C-N-CA	12.60	153.21	121.70
1	I	243	THR	C-N-CA	12.60	153.20	121.70
1	U	243	THR	C-N-CA	12.60	153.20	121.70
1	S	243	THR	C-N-CA	12.60	153.19	121.70
1	e	243	THR	C-N-CA	12.60	153.19	121.70
1	v	243	THR	C-N-CA	12.60	153.19	121.70
1	5	243	THR	C-N-CA	12.60	153.19	121.70
1	y	243	THR	C-N-CA	12.60	153.19	121.70
1	C	243	THR	C-N-CA	12.60	153.19	121.70
1	6	243	THR	C-N-CA	12.59	153.18	121.70
1	7	243	THR	C-N-CA	12.59	153.19	121.70
1	G	243	THR	C-N-CA	12.59	153.18	121.70
1	b	243	THR	C-N-CA	12.59	153.18	121.70
1	R	243	THR	C-N-CA	12.59	153.18	121.70
1	J	243	THR	C-N-CA	12.59	153.17	121.70
1	x	243	THR	C-N-CA	12.59	153.17	121.70
1	2	243	THR	C-N-CA	12.59	153.17	121.70
1	t	243	THR	C-N-CA	12.59	153.17	121.70
1	g	243	THR	C-N-CA	12.59	153.16	121.70
1	j	243	THR	C-N-CA	12.59	153.16	121.70
1	p	243	THR	C-N-CA	12.59	153.16	121.70
1	w	243	THR	C-N-CA	12.59	153.16	121.70
1	a	243	THR	C-N-CA	12.58	153.16	121.70
1	k	243	THR	C-N-CA	12.58	153.16	121.70
1	N	243	THR	C-N-CA	12.58	153.16	121.70
1	4	243	THR	C-N-CA	12.58	153.15	121.70
1	l	243	THR	C-N-CA	12.58	153.15	121.70
1	3	243	THR	C-N-CA	12.57	153.13	121.70
1	u	243	THR	C-N-CA	12.57	153.13	121.70
1	K	243	THR	C-N-CA	12.57	153.13	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	243	THR	C-N-CA	12.57	153.13	121.70
1	B	243	THR	C-N-CA	12.57	153.13	121.70
1	Y	243	THR	C-N-CA	12.57	153.13	121.70
1	1	243	THR	C-N-CA	12.57	153.12	121.70
1	T	243	THR	C-N-CA	12.57	153.12	121.70
1	H	243	THR	C-N-CA	12.57	153.12	121.70
1	f	243	THR	C-N-CA	12.56	153.11	121.70
1	F	258	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	V	258	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	2	258	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	y	258	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	u	258	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	Y	258	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	J	258	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	i	258	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	258	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	n	258	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	5	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	Q	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	d	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	z	258	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	M	258	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	S	258	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	m	258	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	f	258	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	7	258	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	N	258	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	T	258	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	s	258	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	G	258	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	L	258	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	a	258	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	6	258	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	g	258	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	k	258	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	R	258	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	p	258	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	258	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	t	258	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	w	258	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	3	258	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	q	258	ARG	NE-CZ-NH1	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	258	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	e	258	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	b	258	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	W	258	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	c	258	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	Z	258	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	0	258	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	H	258	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	r	258	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	h	258	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	j	258	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	E	258	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	C	258	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	l	258	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	1	258	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	U	258	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	D	258	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	O	258	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	4	258	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	v	258	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	I	258	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	o	258	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	P	258	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	K	258	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	X	258	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	z	92	PRO	N-CA-CB	5.91	110.39	103.30
1	7	92	PRO	N-CA-CB	5.91	110.39	103.30
1	y	92	PRO	N-CA-CB	5.91	110.39	103.30
1	2	92	PRO	N-CA-CB	5.91	110.39	103.30
1	w	92	PRO	N-CA-CB	5.90	110.39	103.30
1	Q	92	PRO	N-CA-CB	5.90	110.38	103.30
1	s	92	PRO	N-CA-CB	5.89	110.37	103.30
1	S	92	PRO	N-CA-CB	5.89	110.37	103.30
1	D	92	PRO	N-CA-CB	5.89	110.37	103.30
1	i	92	PRO	N-CA-CB	5.89	110.37	103.30
1	A	92	PRO	N-CA-CB	5.89	110.37	103.30
1	d	92	PRO	N-CA-CB	5.89	110.36	103.30
1	5	92	PRO	N-CA-CB	5.88	110.36	103.30
1	H	92	PRO	N-CA-CB	5.88	110.36	103.30
1	L	92	PRO	N-CA-CB	5.88	110.36	103.30
1	M	92	PRO	N-CA-CB	5.88	110.36	103.30
1	B	92	PRO	N-CA-CB	5.87	110.35	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	92	PRO	N-CA-CB	5.87	110.34	103.30
1	N	92	PRO	N-CA-CB	5.87	110.34	103.30
1	J	92	PRO	N-CA-CB	5.87	110.34	103.30
1	f	92	PRO	N-CA-CB	5.87	110.34	103.30
1	n	92	PRO	N-CA-CB	5.87	110.34	103.30
1	P	92	PRO	N-CA-CB	5.87	110.34	103.30
1	G	92	PRO	N-CA-CB	5.87	110.34	103.30
1	F	92	PRO	N-CA-CB	5.86	110.34	103.30
1	k	92	PRO	N-CA-CB	5.86	110.33	103.30
1	a	92	PRO	N-CA-CB	5.86	110.33	103.30
1	h	92	PRO	N-CA-CB	5.86	110.33	103.30
1	I	92	PRO	N-CA-CB	5.86	110.33	103.30
1	W	92	PRO	N-CA-CB	5.86	110.33	103.30
1	R	92	PRO	N-CA-CB	5.86	110.33	103.30
1	0	92	PRO	N-CA-CB	5.85	110.33	103.30
1	p	92	PRO	N-CA-CB	5.85	110.32	103.30
1	c	92	PRO	N-CA-CB	5.85	110.32	103.30
1	e	92	PRO	N-CA-CB	5.85	110.32	103.30
1	T	92	PRO	N-CA-CB	5.85	110.32	103.30
1	C	92	PRO	N-CA-CB	5.85	110.32	103.30
1	t	92	PRO	N-CA-CB	5.85	110.32	103.30
1	l	92	PRO	N-CA-CB	5.85	110.32	103.30
1	o	92	PRO	N-CA-CB	5.85	110.31	103.30
1	V	92	PRO	N-CA-CB	5.85	110.31	103.30
1	j	92	PRO	N-CA-CB	5.84	110.31	103.30
1	E	92	PRO	N-CA-CB	5.84	110.31	103.30
1	b	92	PRO	N-CA-CB	5.84	110.31	103.30
1	g	92	PRO	N-CA-CB	5.84	110.31	103.30
1	Y	92	PRO	N-CA-CB	5.84	110.31	103.30
1	K	92	PRO	N-CA-CB	5.84	110.31	103.30
1	m	92	PRO	N-CA-CB	5.84	110.31	103.30
1	r	92	PRO	N-CA-CB	5.84	110.31	103.30
1	O	92	PRO	N-CA-CB	5.83	110.30	103.30
1	v	92	PRO	N-CA-CB	5.83	110.30	103.30
1	l	92	PRO	N-CA-CB	5.83	110.30	103.30
1	Z	92	PRO	N-CA-CB	5.83	110.30	103.30
1	3	92	PRO	N-CA-CB	5.83	110.29	103.30
1	U	92	PRO	N-CA-CB	5.83	110.29	103.30
1	X	92	PRO	N-CA-CB	5.83	110.29	103.30
1	u	92	PRO	N-CA-CB	5.82	110.29	103.30
1	6	92	PRO	N-CA-CB	5.82	110.28	103.30
1	q	92	PRO	N-CA-CB	5.82	110.28	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	x	92	PRO	N-CA-CB	5.81	110.28	103.30
1	W	130	PRO	N-CA-CB	5.27	109.62	103.30
1	S	130	PRO	N-CA-CB	5.26	109.61	103.30
1	A	130	PRO	N-CA-CB	5.26	109.61	103.30
1	Q	130	PRO	N-CA-CB	5.26	109.61	103.30
1	Z	130	PRO	N-CA-CB	5.26	109.61	103.30
1	n	130	PRO	N-CA-CB	5.26	109.61	103.30
1	V	130	PRO	N-CA-CB	5.26	109.61	103.30
1	5	130	PRO	N-CA-CB	5.25	109.60	103.30
1	T	130	PRO	N-CA-CB	5.25	109.60	103.30
1	M	130	PRO	N-CA-CB	5.25	109.60	103.30
1	i	130	PRO	N-CA-CB	5.25	109.60	103.30
1	D	130	PRO	N-CA-CB	5.25	109.60	103.30
1	j	130	PRO	N-CA-CB	5.25	109.59	103.30
1	d	130	PRO	N-CA-CB	5.25	109.59	103.30
1	s	130	PRO	N-CA-CB	5.25	109.59	103.30
1	B	130	PRO	N-CA-CB	5.24	109.59	103.30
1	q	130	PRO	N-CA-CB	5.24	109.59	103.30
1	w	130	PRO	N-CA-CB	5.24	109.59	103.30
1	g	130	PRO	N-CA-CB	5.24	109.58	103.30
1	X	130	PRO	N-CA-CB	5.24	109.58	103.30
1	4	130	PRO	N-CA-CB	5.23	109.58	103.30
1	7	130	PRO	N-CA-CB	5.23	109.58	103.30
1	z	130	PRO	N-CA-CB	5.23	109.58	103.30
1	h	130	PRO	N-CA-CB	5.23	109.57	103.30
1	m	130	PRO	N-CA-CB	5.23	109.57	103.30
1	a	130	PRO	N-CA-CB	5.22	109.57	103.30
1	F	130	PRO	N-CA-CB	5.22	109.57	103.30
1	b	130	PRO	N-CA-CB	5.22	109.57	103.30
1	K	130	PRO	N-CA-CB	5.22	109.57	103.30
1	x	130	PRO	N-CA-CB	5.22	109.57	103.30
1	Y	130	PRO	N-CA-CB	5.22	109.57	103.30
1	o	130	PRO	N-CA-CB	5.22	109.56	103.30
1	y	130	PRO	N-CA-CB	5.22	109.56	103.30
1	0	130	PRO	N-CA-CB	5.22	109.56	103.30
1	R	130	PRO	N-CA-CB	5.22	109.56	103.30
1	L	130	PRO	N-CA-CB	5.21	109.56	103.30
1	k	130	PRO	N-CA-CB	5.21	109.56	103.30
1	I	130	PRO	N-CA-CB	5.21	109.56	103.30
1	J	130	PRO	N-CA-CB	5.21	109.55	103.30
1	c	130	PRO	N-CA-CB	5.21	109.55	103.30
1	u	130	PRO	N-CA-CB	5.21	109.55	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	130	PRO	N-CA-CB	5.21	109.55	103.30
1	e	130	PRO	N-CA-CB	5.20	109.54	103.30
1	l	130	PRO	N-CA-CB	5.20	109.55	103.30
1	p	130	PRO	N-CA-CB	5.20	109.54	103.30
1	t	130	PRO	N-CA-CB	5.20	109.54	103.30
1	1	130	PRO	N-CA-CB	5.20	109.54	103.30
1	v	130	PRO	N-CA-CB	5.20	109.53	103.30
1	H	130	PRO	N-CA-CB	5.20	109.53	103.30
1	f	130	PRO	N-CA-CB	5.19	109.53	103.30
1	3	130	PRO	N-CA-CB	5.19	109.53	103.30
1	N	130	PRO	N-CA-CB	5.19	109.53	103.30
1	E	130	PRO	N-CA-CB	5.19	109.53	103.30
1	6	130	PRO	N-CA-CB	5.19	109.53	103.30
1	r	130	PRO	N-CA-CB	5.19	109.52	103.30
1	G	130	PRO	N-CA-CB	5.19	109.52	103.30
1	U	130	PRO	N-CA-CB	5.18	109.52	103.30
1	2	130	PRO	N-CA-CB	5.18	109.52	103.30
1	P	130	PRO	N-CA-CB	5.17	109.51	103.30
1	C	130	PRO	N-CA-CB	5.14	109.47	103.30
1	P	390	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	N	390	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	h	390	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	F	390	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	q	390	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	X	390	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	l	390	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	6	390	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	b	390	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	T	390	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	G	390	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	y	390	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	7	390	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	U	390	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	g	390	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	D	390	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	j	390	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	c	390	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	e	390	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	2	390	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	w	390	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	R	390	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	o	390	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	390	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	r	390	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	i	390	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	s	390	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	1	390	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	243	THR	Peptide,Mainchain
1	1	243	THR	Peptide,Mainchain
1	2	243	THR	Peptide,Mainchain
1	3	243	THR	Peptide,Mainchain
1	4	243	THR	Peptide,Mainchain
1	5	243	THR	Peptide,Mainchain
1	6	243	THR	Peptide,Mainchain
1	7	243	THR	Peptide,Mainchain
1	A	243	THR	Peptide,Mainchain
1	B	243	THR	Peptide,Mainchain
1	C	243	THR	Peptide,Mainchain
1	D	243	THR	Peptide,Mainchain
1	E	243	THR	Peptide,Mainchain
1	F	243	THR	Peptide,Mainchain
1	G	243	THR	Peptide,Mainchain
1	H	243	THR	Peptide,Mainchain
1	I	243	THR	Peptide,Mainchain
1	J	243	THR	Peptide,Mainchain
1	K	243	THR	Peptide,Mainchain
1	L	243	THR	Peptide,Mainchain
1	M	243	THR	Peptide,Mainchain
1	N	243	THR	Peptide,Mainchain
1	O	243	THR	Peptide,Mainchain
1	P	243	THR	Peptide,Mainchain
1	Q	243	THR	Peptide,Mainchain
1	R	243	THR	Peptide,Mainchain
1	S	243	THR	Peptide,Mainchain
1	T	243	THR	Peptide,Mainchain
1	U	243	THR	Peptide,Mainchain
1	V	243	THR	Peptide,Mainchain
1	W	243	THR	Peptide,Mainchain
1	X	243	THR	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	Y	243	THR	Peptide,Mainchain
1	Z	243	THR	Peptide,Mainchain
1	a	243	THR	Peptide,Mainchain
1	b	243	THR	Peptide,Mainchain
1	c	243	THR	Peptide,Mainchain
1	d	243	THR	Peptide,Mainchain
1	e	243	THR	Peptide,Mainchain
1	f	243	THR	Peptide,Mainchain
1	g	243	THR	Peptide,Mainchain
1	h	243	THR	Peptide,Mainchain
1	i	243	THR	Peptide,Mainchain
1	j	243	THR	Peptide,Mainchain
1	k	243	THR	Peptide,Mainchain
1	l	243	THR	Peptide,Mainchain
1	m	243	THR	Peptide,Mainchain
1	n	243	THR	Peptide,Mainchain
1	o	243	THR	Peptide,Mainchain
1	p	243	THR	Peptide,Mainchain
1	q	243	THR	Peptide,Mainchain
1	r	243	THR	Peptide,Mainchain
1	s	243	THR	Peptide,Mainchain
1	t	243	THR	Peptide,Mainchain
1	u	243	THR	Peptide,Mainchain
1	v	243	THR	Peptide,Mainchain
1	w	243	THR	Peptide,Mainchain
1	x	243	THR	Peptide,Mainchain
1	y	243	THR	Peptide,Mainchain
1	z	243	THR	Peptide,Mainchain

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	1	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	2	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	3	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	4	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	5	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	6	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	7	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	A	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	B	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	C	488/672 (73%)	451 (92%)	33 (7%)	4 (1%)	16	52
1	D	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	E	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	F	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	G	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	H	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	I	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	J	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	K	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	L	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	M	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	N	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	O	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	P	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	Q	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	R	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	S	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	T	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	U	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	V	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	W	488/672 (73%)	451 (92%)	33 (7%)	4 (1%)	16	52
1	X	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	Y	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	Z	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	a	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	b	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	c	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	d	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	e	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	f	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	g	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	h	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	i	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	j	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	k	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	l	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	m	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	n	488/672 (73%)	451 (92%)	33 (7%)	4 (1%)	16	52
1	o	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	p	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	q	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	r	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	s	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	t	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	u	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	v	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	w	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	x	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	y	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
1	z	488/672 (73%)	450 (92%)	34 (7%)	4 (1%)	16	52
All	All	29280/40320 (73%)	27003 (92%)	2037 (7%)	240 (1%)	19	52

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	240	GLN
1	0	450	VAL
1	a	240	GLN
1	a	450	VAL
1	b	240	GLN
1	b	450	VAL
1	c	240	GLN
1	c	450	VAL
1	d	240	GLN
1	d	450	VAL
1	3	240	GLN
1	3	450	VAL
1	4	240	GLN
1	4	450	VAL
1	5	240	GLN
1	5	450	VAL
1	6	240	GLN
1	6	450	VAL
1	7	240	GLN
1	7	450	VAL
1	I	240	GLN
1	I	450	VAL
1	J	240	GLN
1	J	450	VAL
1	K	240	GLN
1	K	450	VAL
1	L	240	GLN
1	L	450	VAL
1	M	240	GLN
1	M	450	VAL
1	e	240	GLN
1	e	450	VAL
1	f	240	GLN
1	f	450	VAL
1	g	240	GLN
1	g	450	VAL
1	h	240	GLN
1	h	450	VAL
1	i	240	GLN
1	i	450	VAL
1	j	240	GLN
1	j	450	VAL

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Mol	Chain	Res	Type
1	k	240	GLN
1	k	450	VAL
1	l	240	GLN
1	l	450	VAL
1	m	240	GLN
1	m	450	VAL
1	n	240	GLN
1	n	450	VAL
1	o	240	GLN
1	o	450	VAL
1	p	240	GLN
1	p	450	VAL
1	q	240	GLN
1	q	450	VAL
1	r	240	GLN
1	r	450	VAL
1	s	240	GLN
1	s	450	VAL
1	t	240	GLN
1	t	450	VAL
1	u	240	GLN
1	u	450	VAL
1	v	240	GLN
1	v	450	VAL
1	w	240	GLN
1	w	450	VAL
1	x	240	GLN
1	x	450	VAL
1	y	240	GLN
1	y	450	VAL
1	1	240	GLN
1	1	450	VAL
1	2	240	GLN
1	2	450	VAL
1	O	240	GLN
1	O	450	VAL
1	z	240	GLN
1	z	450	VAL
1	A	240	GLN
1	A	450	VAL
1	B	240	GLN
1	B	450	VAL

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Mol	Chain	Res	Type
1	D	240	GLN
1	D	450	VAL
1	E	240	GLN
1	E	450	VAL
1	F	240	GLN
1	F	450	VAL
1	G	240	GLN
1	G	450	VAL
1	H	240	GLN
1	H	450	VAL
1	N	240	GLN
1	N	450	VAL
1	P	240	GLN
1	P	450	VAL
1	Q	240	GLN
1	Q	450	VAL
1	R	240	GLN
1	R	450	VAL
1	T	240	GLN
1	T	450	VAL
1	U	240	GLN
1	U	450	VAL
1	V	240	GLN
1	V	450	VAL
1	W	240	GLN
1	W	450	VAL
1	X	240	GLN
1	X	450	VAL
1	Y	240	GLN
1	Y	450	VAL
1	Z	240	GLN
1	Z	450	VAL
1	C	240	GLN
1	C	450	VAL
1	S	240	GLN
1	S	450	VAL
1	0	400	ARG
1	a	400	ARG
1	b	400	ARG
1	c	400	ARG
1	d	400	ARG
1	3	400	ARG

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Mol	Chain	Res	Type
1	4	400	ARG
1	5	400	ARG
1	6	400	ARG
1	7	400	ARG
1	I	400	ARG
1	J	400	ARG
1	K	400	ARG
1	L	400	ARG
1	M	400	ARG
1	e	400	ARG
1	f	400	ARG
1	g	400	ARG
1	h	400	ARG
1	i	400	ARG
1	j	400	ARG
1	k	400	ARG
1	l	400	ARG
1	m	400	ARG
1	n	400	ARG
1	o	400	ARG
1	p	400	ARG
1	q	400	ARG
1	r	400	ARG
1	s	400	ARG
1	t	400	ARG
1	u	400	ARG
1	v	400	ARG
1	w	400	ARG
1	x	400	ARG
1	y	400	ARG
1	1	400	ARG
1	2	400	ARG
1	O	400	ARG
1	z	400	ARG
1	A	400	ARG
1	B	400	ARG
1	D	400	ARG
1	E	400	ARG
1	F	400	ARG
1	G	400	ARG
1	H	400	ARG
1	N	400	ARG

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Mol	Chain	Res	Type
1	P	400	ARG
1	Q	400	ARG
1	R	400	ARG
1	T	400	ARG
1	U	400	ARG
1	V	400	ARG
1	W	400	ARG
1	X	400	ARG
1	Y	400	ARG
1	Z	400	ARG
1	C	400	ARG
1	S	400	ARG
1	0	237	GLY
1	a	237	GLY
1	b	237	GLY
1	c	237	GLY
1	d	237	GLY
1	3	237	GLY
1	4	237	GLY
1	5	237	GLY
1	6	237	GLY
1	7	237	GLY
1	I	237	GLY
1	J	237	GLY
1	K	237	GLY
1	L	237	GLY
1	M	237	GLY
1	e	237	GLY
1	f	237	GLY
1	h	237	GLY
1	i	237	GLY
1	j	237	GLY
1	k	237	GLY
1	l	237	GLY
1	m	237	GLY
1	n	237	GLY
1	o	237	GLY
1	p	237	GLY
1	q	237	GLY
1	r	237	GLY
1	s	237	GLY
1	t	237	GLY

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Mol	Chain	Res	Type
1	u	237	GLY
1	v	237	GLY
1	w	237	GLY
1	x	237	GLY
1	y	237	GLY
1	1	237	GLY
1	2	237	GLY
1	O	237	GLY
1	z	237	GLY
1	A	237	GLY
1	B	237	GLY
1	D	237	GLY
1	E	237	GLY
1	F	237	GLY
1	G	237	GLY
1	H	237	GLY
1	P	237	GLY
1	Q	237	GLY
1	R	237	GLY
1	T	237	GLY
1	U	237	GLY
1	V	237	GLY
1	W	237	GLY
1	X	237	GLY
1	Y	237	GLY
1	Z	237	GLY
1	C	237	GLY
1	S	237	GLY
1	g	237	GLY
1	N	237	GLY

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	0	422/629 (67%)	420 (100%)	2 (0%)	86 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	2	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	3	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	4	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	5	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	6	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	7	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	A	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	B	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	C	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	D	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	E	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	F	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	G	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	H	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	I	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	J	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	K	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	L	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	M	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	N	421/629 (67%)	419 (100%)	2 (0%)	86	90
1	O	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	P	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	Q	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	R	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	S	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	T	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	U	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	V	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	W	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	X	422/629 (67%)	420 (100%)	2 (0%)	86	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Y	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	Z	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	a	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	b	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	c	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	d	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	e	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	f	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	g	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	h	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	i	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	j	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	k	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	l	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	m	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	n	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	o	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	p	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	q	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	r	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	s	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	t	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	u	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	v	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	w	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	x	422/629 (67%)	420 (100%)	2 (0%)	86	90
1	y	421/629 (67%)	419 (100%)	2 (0%)	86	90
1	z	422/629 (67%)	420 (100%)	2 (0%)	86	90
All	All	25318/37740 (67%)	25198 (100%)	120 (0%)	85	90

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	236	ILE
1	0	259	ASP
1	a	236	ILE
1	a	259	ASP
1	b	236	ILE
1	b	259	ASP
1	c	236	ILE
1	c	259	ASP
1	d	236	ILE
1	d	259	ASP
1	3	236	ILE
1	3	259	ASP
1	4	236	ILE
1	4	259	ASP
1	5	236	ILE
1	5	259	ASP
1	6	236	ILE
1	6	259	ASP
1	7	236	ILE
1	7	259	ASP
1	I	236	ILE
1	I	259	ASP
1	J	236	ILE
1	J	259	ASP
1	K	236	ILE
1	K	259	ASP
1	L	236	ILE
1	L	259	ASP
1	M	236	ILE
1	M	259	ASP
1	e	236	ILE
1	e	259	ASP
1	f	236	ILE
1	f	259	ASP
1	g	236	ILE
1	g	259	ASP
1	h	236	ILE
1	h	259	ASP
1	i	236	ILE
1	i	259	ASP
1	j	236	ILE
1	j	259	ASP
1	k	236	ILE

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Mol	Chain	Res	Type
1	k	259	ASP
1	l	236	ILE
1	l	259	ASP
1	m	236	ILE
1	m	259	ASP
1	n	236	ILE
1	n	259	ASP
1	o	236	ILE
1	o	259	ASP
1	p	236	ILE
1	p	259	ASP
1	q	236	ILE
1	q	259	ASP
1	r	236	ILE
1	r	259	ASP
1	s	236	ILE
1	s	259	ASP
1	t	236	ILE
1	t	259	ASP
1	u	236	ILE
1	u	259	ASP
1	v	236	ILE
1	v	259	ASP
1	w	236	ILE
1	w	259	ASP
1	x	236	ILE
1	x	259	ASP
1	y	236	ILE
1	y	259	ASP
1	1	236	ILE
1	1	259	ASP
1	2	236	ILE
1	2	259	ASP
1	O	236	ILE
1	O	259	ASP
1	z	236	ILE
1	z	259	ASP
1	A	236	ILE
1	A	259	ASP
1	B	236	ILE
1	B	259	ASP
1	D	236	ILE

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Mol	Chain	Res	Type
1	D	259	ASP
1	E	236	ILE
1	E	259	ASP
1	F	236	ILE
1	F	259	ASP
1	G	236	ILE
1	G	259	ASP
1	H	236	ILE
1	H	259	ASP
1	N	236	ILE
1	N	259	ASP
1	P	236	ILE
1	P	259	ASP
1	Q	236	ILE
1	Q	259	ASP
1	R	236	ILE
1	R	259	ASP
1	T	236	ILE
1	T	259	ASP
1	U	236	ILE
1	U	259	ASP
1	V	236	ILE
1	V	259	ASP
1	W	236	ILE
1	W	259	ASP
1	X	236	ILE
1	X	259	ASP
1	Y	236	ILE
1	Y	259	ASP
1	Z	236	ILE
1	Z	259	ASP
1	C	236	ILE
1	C	259	ASP
1	S	236	ILE
1	S	259	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	275	GLN
1	0	512	ASN
1	a	275	GLN

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Mol	Chain	Res	Type
1	a	512	ASN
1	b	275	GLN
1	b	351	ASN
1	b	512	ASN
1	c	275	GLN
1	c	351	ASN
1	c	512	ASN
1	d	275	GLN
1	d	512	ASN
1	3	275	GLN
1	3	351	ASN
1	3	512	ASN
1	4	275	GLN
1	4	351	ASN
1	4	512	ASN
1	5	275	GLN
1	5	351	ASN
1	5	512	ASN
1	6	275	GLN
1	6	512	ASN
1	7	275	GLN
1	7	512	ASN
1	I	275	GLN
1	I	351	ASN
1	I	512	ASN
1	J	275	GLN
1	J	512	ASN
1	K	275	GLN
1	K	512	ASN
1	L	275	GLN
1	L	351	ASN
1	L	512	ASN
1	M	275	GLN
1	M	351	ASN
1	M	512	ASN
1	e	275	GLN
1	e	351	ASN
1	e	512	ASN
1	f	275	GLN
1	f	351	ASN
1	f	512	ASN
1	g	275	GLN

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Mol	Chain	Res	Type
1	g	512	ASN
1	h	275	GLN
1	h	351	ASN
1	h	512	ASN
1	i	275	GLN
1	i	512	ASN
1	j	275	GLN
1	j	512	ASN
1	k	275	GLN
1	k	512	ASN
1	l	275	GLN
1	l	351	ASN
1	l	512	ASN
1	m	275	GLN
1	m	351	ASN
1	m	512	ASN
1	n	275	GLN
1	n	351	ASN
1	n	512	ASN
1	o	275	GLN
1	o	512	ASN
1	p	275	GLN
1	p	512	ASN
1	q	275	GLN
1	q	351	ASN
1	q	512	ASN
1	r	209	GLN
1	r	275	GLN
1	r	351	ASN
1	r	512	ASN
1	s	275	GLN
1	s	512	ASN
1	t	275	GLN
1	t	512	ASN
1	u	275	GLN
1	u	512	ASN
1	v	275	GLN
1	v	512	ASN
1	w	275	GLN
1	w	512	ASN
1	x	275	GLN
1	x	351	ASN

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Mol	Chain	Res	Type
1	x	512	ASN
1	y	275	GLN
1	y	512	ASN
1	1	275	GLN
1	1	512	ASN
1	2	275	GLN
1	2	351	ASN
1	2	512	ASN
1	O	275	GLN
1	O	351	ASN
1	O	512	ASN
1	z	275	GLN
1	z	351	ASN
1	z	512	ASN
1	A	275	GLN
1	A	512	ASN
1	B	275	GLN
1	B	512	ASN
1	D	275	GLN
1	D	351	ASN
1	D	512	ASN
1	E	275	GLN
1	E	351	ASN
1	E	512	ASN
1	F	275	GLN
1	F	512	ASN
1	G	275	GLN
1	G	512	ASN
1	H	275	GLN
1	H	351	ASN
1	H	512	ASN
1	N	275	GLN
1	N	351	ASN
1	N	512	ASN
1	P	275	GLN
1	P	351	ASN
1	P	512	ASN
1	Q	275	GLN
1	Q	351	ASN
1	Q	512	ASN
1	R	275	GLN
1	R	512	ASN

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Mol	Chain	Res	Type
1	T	275	GLN
1	T	351	ASN
1	T	512	ASN
1	U	275	GLN
1	U	351	ASN
1	U	512	ASN
1	V	275	GLN
1	V	351	ASN
1	V	512	ASN
1	W	275	GLN
1	W	351	ASN
1	W	512	ASN
1	X	275	GLN
1	X	512	ASN
1	Y	275	GLN
1	Y	351	ASN
1	Y	512	ASN
1	Z	275	GLN
1	Z	351	ASN
1	Z	512	ASN
1	C	275	GLN
1	C	512	ASN
1	S	275	GLN
1	S	512	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	0	1
1	a	1
1	b	1
1	c	1
1	d	1
1	3	1
1	4	1
1	5	1
1	6	1
1	7	1
1	I	1
1	J	1
1	K	1
1	L	1
1	M	1
1	e	1
1	f	1
1	g	1
1	h	1
1	i	1
1	j	1
1	k	1
1	l	1
1	m	1
1	n	1
1	o	1
1	p	1
1	q	1
1	r	1
1	s	1
1	t	1
1	u	1
1	v	1
1	w	1
1	x	1

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Mol	Chain	Number of breaks
1	y	1
1	1	1
1	2	1
1	O	1
1	z	1
1	A	1
1	B	1
1	D	1
1	E	1
1	F	1
1	G	1
1	H	1
1	N	1
1	P	1
1	Q	1
1	R	1
1	T	1
1	U	1
1	V	1
1	W	1
1	X	1
1	Y	1
1	Z	1
1	C	1
1	S	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0	243:THR	C	244:ASN	N	1.08
1	a	243:THR	C	244:ASN	N	1.08
1	b	243:THR	C	244:ASN	N	1.08
1	c	243:THR	C	244:ASN	N	1.08
1	d	243:THR	C	244:ASN	N	1.08
1	3	243:THR	C	244:ASN	N	1.08
1	4	243:THR	C	244:ASN	N	1.08
1	5	243:THR	C	244:ASN	N	1.08
1	6	243:THR	C	244:ASN	N	1.08
1	7	243:THR	C	244:ASN	N	1.08
1	I	243:THR	C	244:ASN	N	1.08
1	J	243:THR	C	244:ASN	N	1.08
1	K	243:THR	C	244:ASN	N	1.08
1	L	243:THR	C	244:ASN	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	243:THR	C	244:ASN	N	1.08
1	e	243:THR	C	244:ASN	N	1.08
1	f	243:THR	C	244:ASN	N	1.08
1	g	243:THR	C	244:ASN	N	1.08
1	h	243:THR	C	244:ASN	N	1.08
1	i	243:THR	C	244:ASN	N	1.08
1	j	243:THR	C	244:ASN	N	1.08
1	k	243:THR	C	244:ASN	N	1.08
1	l	243:THR	C	244:ASN	N	1.08
1	m	243:THR	C	244:ASN	N	1.08
1	n	243:THR	C	244:ASN	N	1.08
1	o	243:THR	C	244:ASN	N	1.08
1	p	243:THR	C	244:ASN	N	1.08
1	q	243:THR	C	244:ASN	N	1.08
1	r	243:THR	C	244:ASN	N	1.08
1	s	243:THR	C	244:ASN	N	1.08
1	t	243:THR	C	244:ASN	N	1.08
1	u	243:THR	C	244:ASN	N	1.08
1	v	243:THR	C	244:ASN	N	1.08
1	w	243:THR	C	244:ASN	N	1.08
1	x	243:THR	C	244:ASN	N	1.08
1	y	243:THR	C	244:ASN	N	1.08
1	1	243:THR	C	244:ASN	N	1.08
1	2	243:THR	C	244:ASN	N	1.08
1	O	243:THR	C	244:ASN	N	1.08
1	z	243:THR	C	244:ASN	N	1.08
1	A	243:THR	C	244:ASN	N	1.08
1	B	243:THR	C	244:ASN	N	1.08
1	D	243:THR	C	244:ASN	N	1.08
1	E	243:THR	C	244:ASN	N	1.08
1	F	243:THR	C	244:ASN	N	1.08
1	G	243:THR	C	244:ASN	N	1.08
1	H	243:THR	C	244:ASN	N	1.08
1	N	243:THR	C	244:ASN	N	1.08
1	P	243:THR	C	244:ASN	N	1.08
1	Q	243:THR	C	244:ASN	N	1.08
1	R	243:THR	C	244:ASN	N	1.08
1	T	243:THR	C	244:ASN	N	1.08
1	U	243:THR	C	244:ASN	N	1.08
1	V	243:THR	C	244:ASN	N	1.08
1	W	243:THR	C	244:ASN	N	1.08
1	X	243:THR	C	244:ASN	N	1.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	243:THR	C	244:ASN	N	1.08
1	Z	243:THR	C	244:ASN	N	1.08
1	C	243:THR	C	244:ASN	N	1.08
1	S	243:THR	C	244:ASN	N	1.08

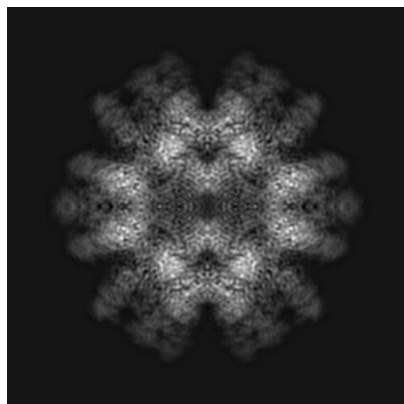
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27077. These allow visual inspection of the internal detail of the map and identification of artifacts.

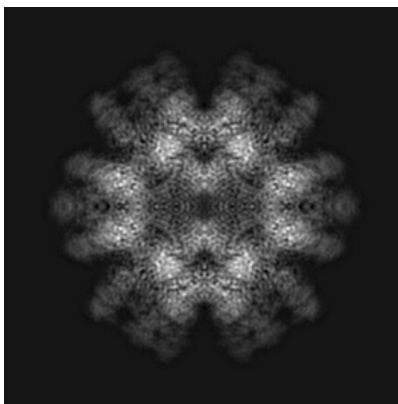
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

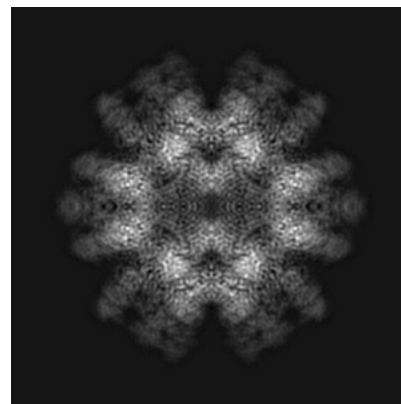
6.1.1 Primary map



X

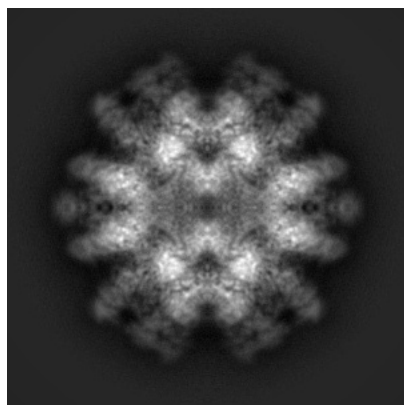


Y

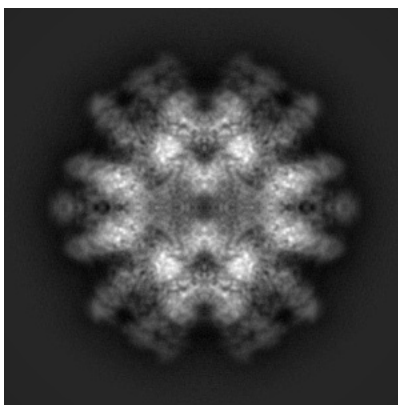


Z

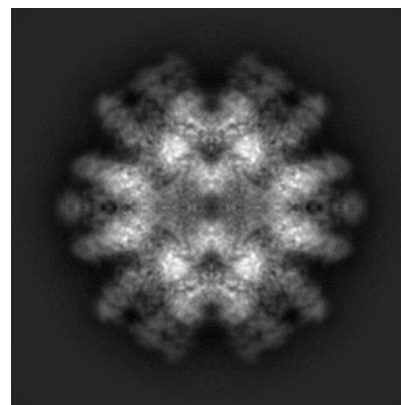
6.1.2 Raw map



X



Y

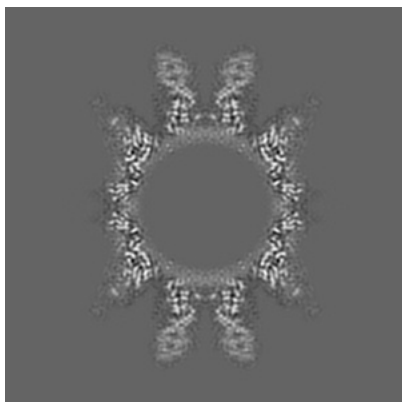


Z

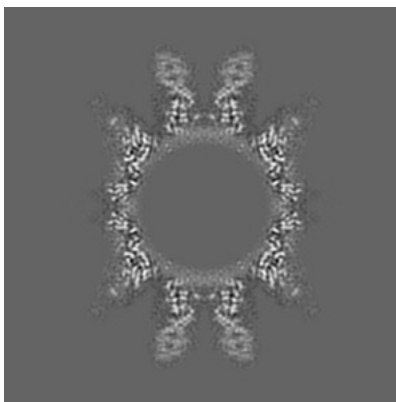
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

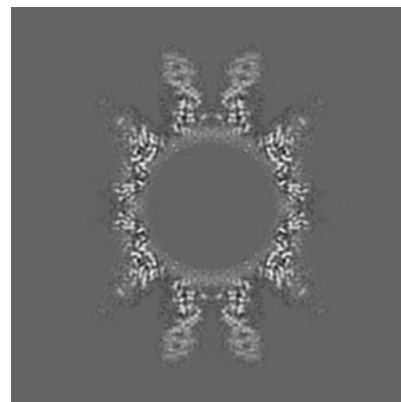
6.2.1 Primary map



X Index: 220

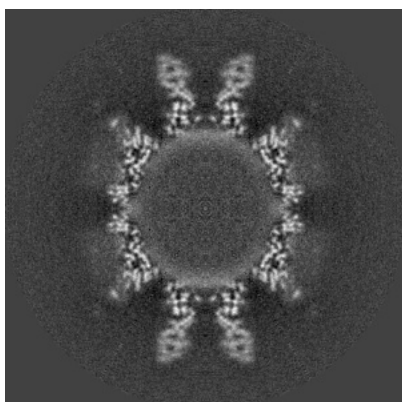


Y Index: 220

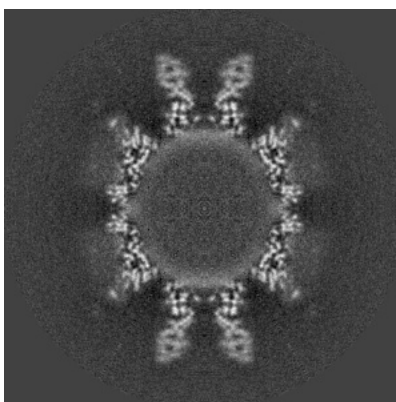


Z Index: 220

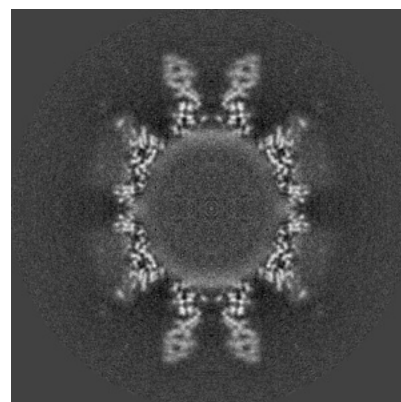
6.2.2 Raw map



X Index: 220



Y Index: 220

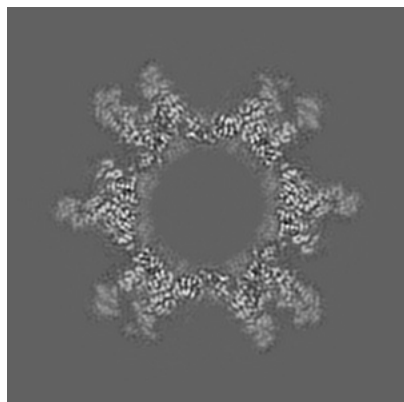


Z Index: 220

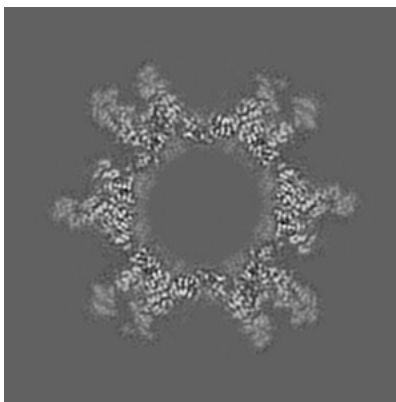
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

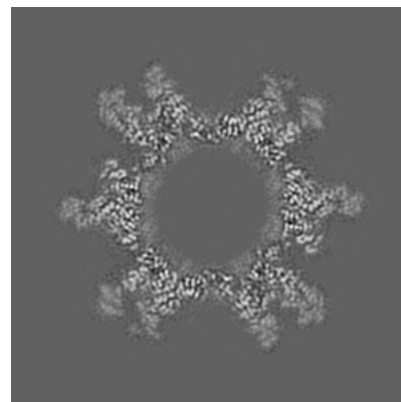
6.3.1 Primary map



X Index: 187

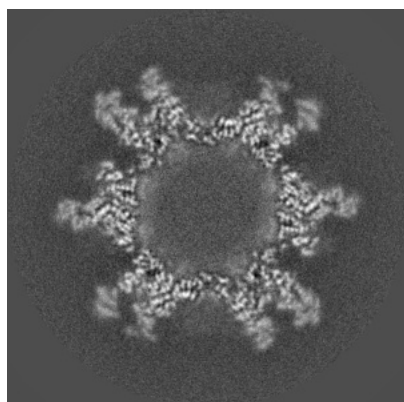


Y Index: 187

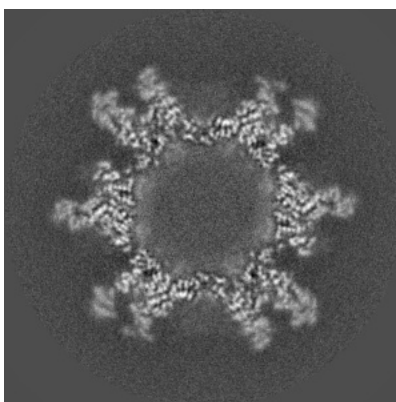


Z Index: 187

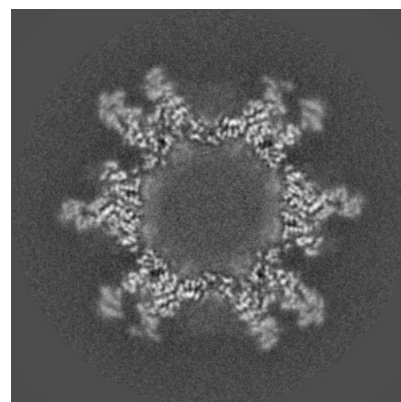
6.3.2 Raw map



X Index: 187



Y Index: 187

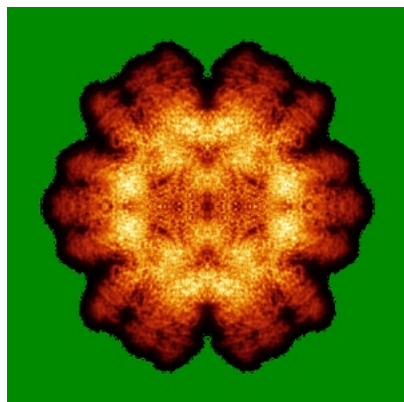


Z Index: 187

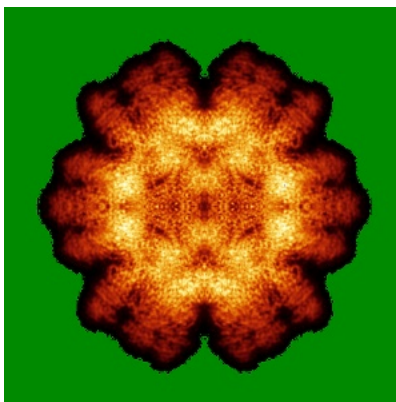
The images above show the largest variance slices of the map in three orthogonal directions.

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

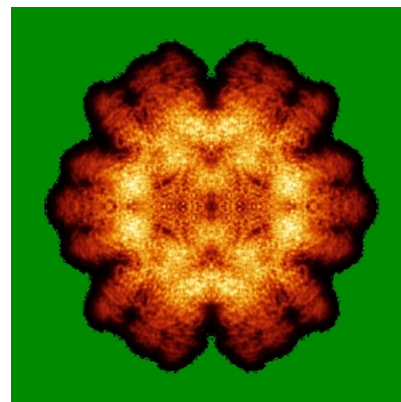
6.4.1 Primary map



X

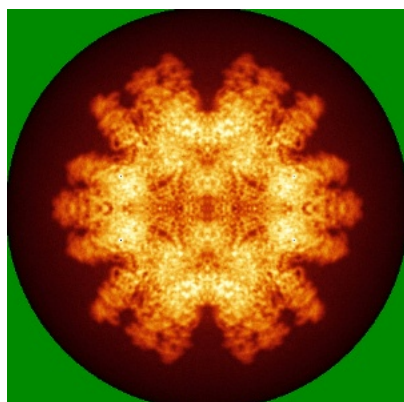


Y

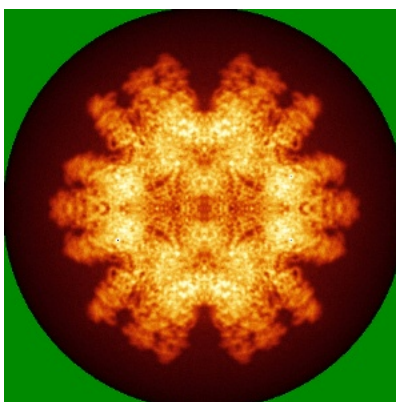


Z

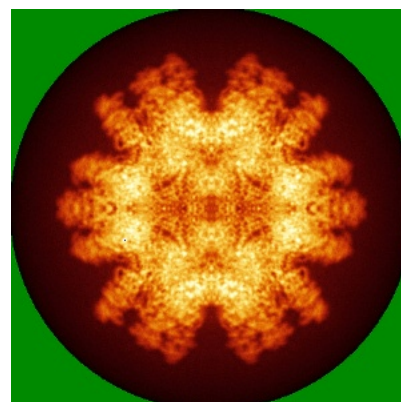
6.4.2 Raw map



X



Y

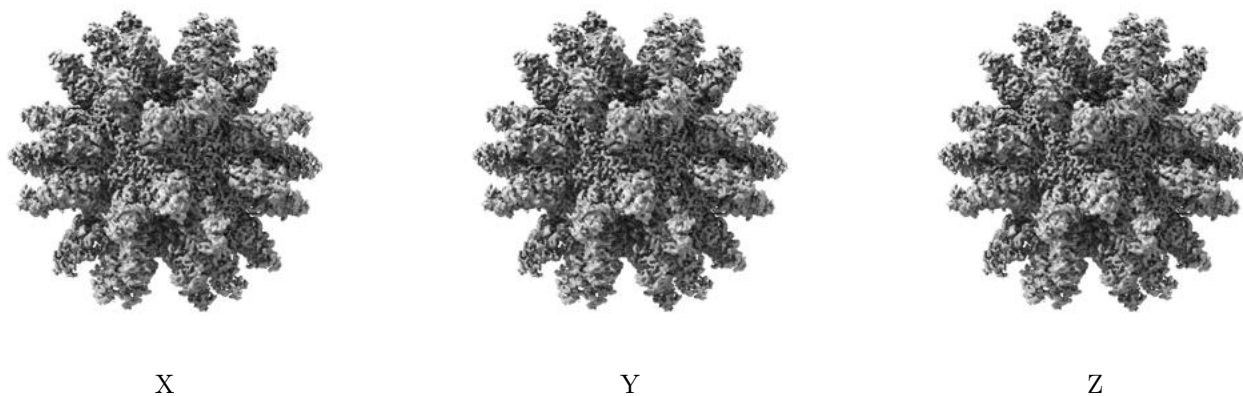


Z

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

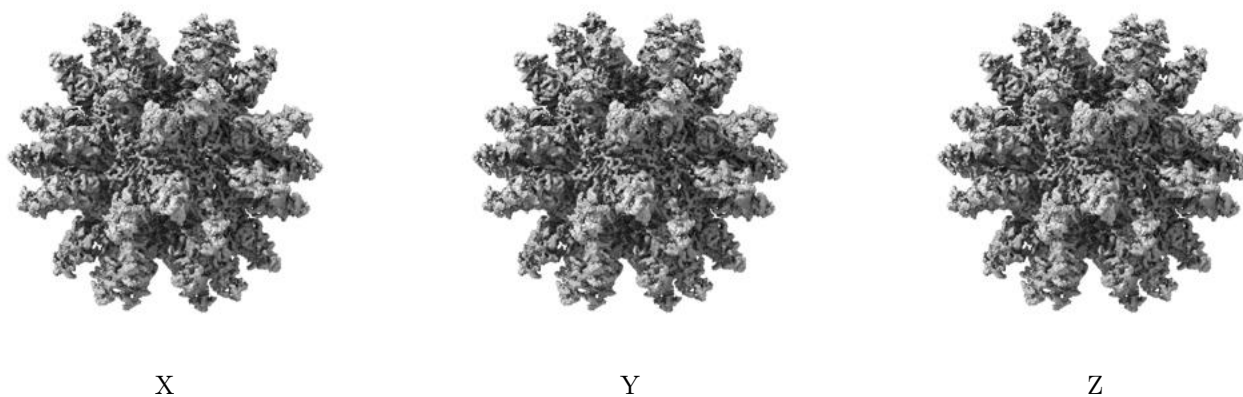
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.87. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

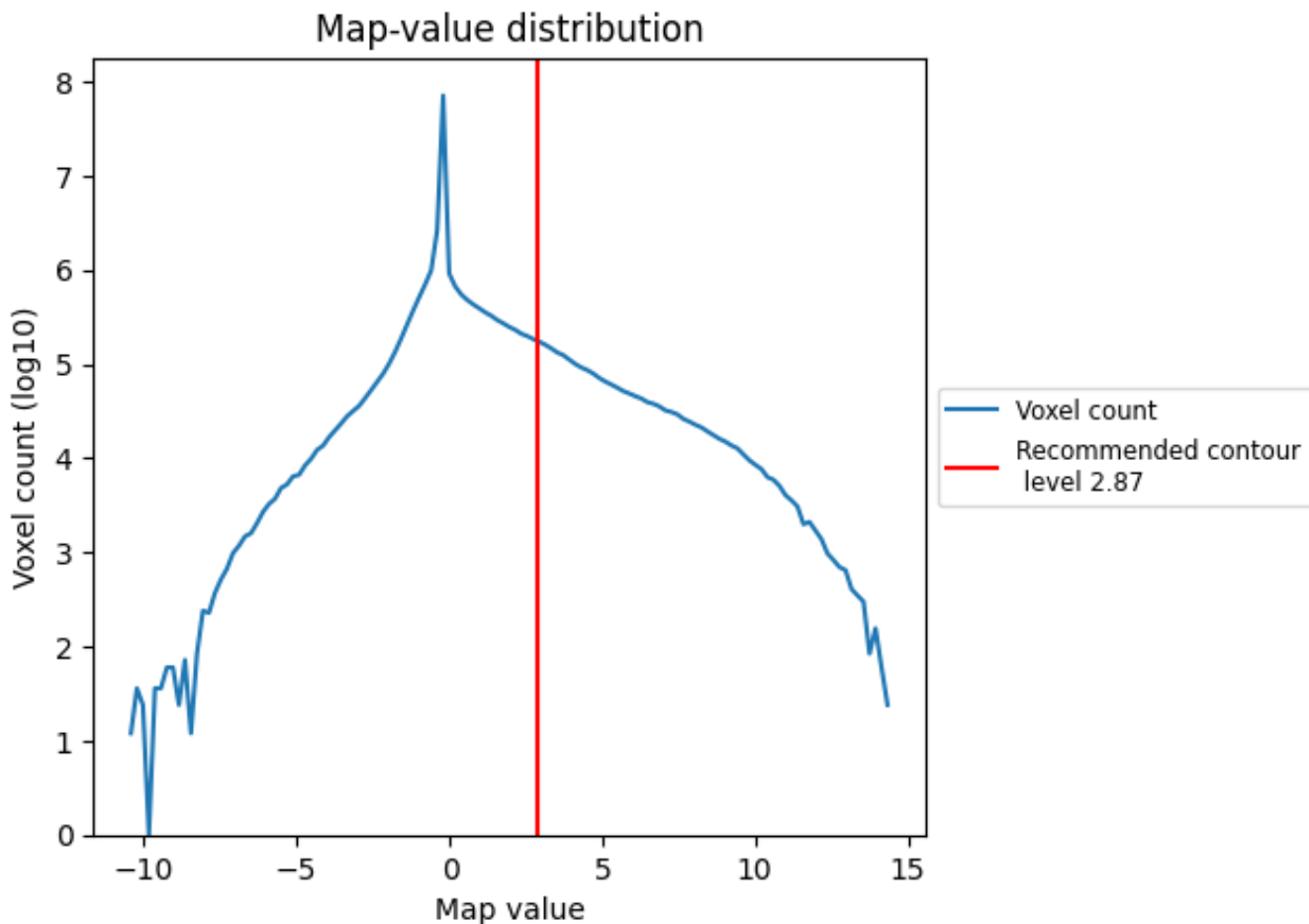
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

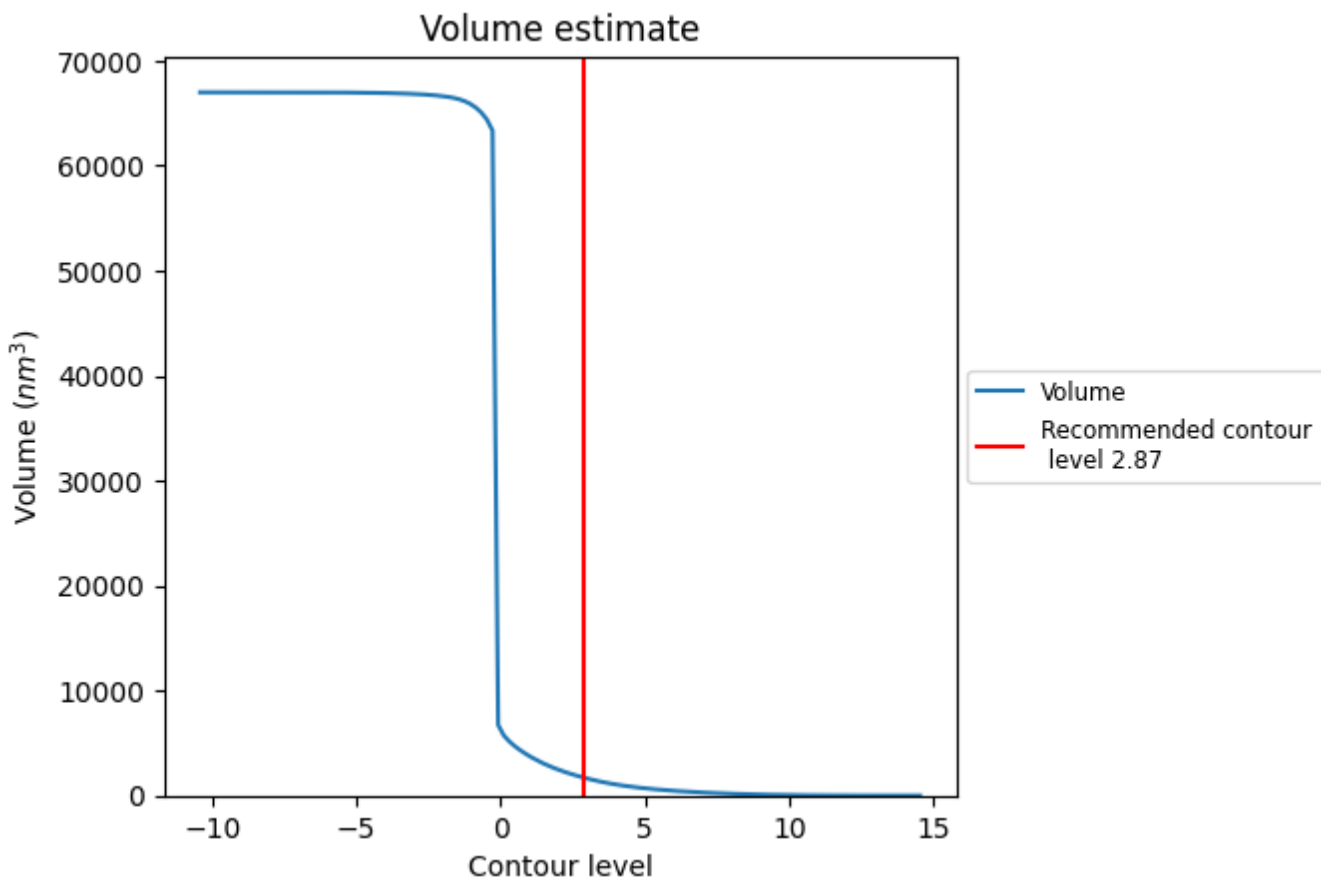
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

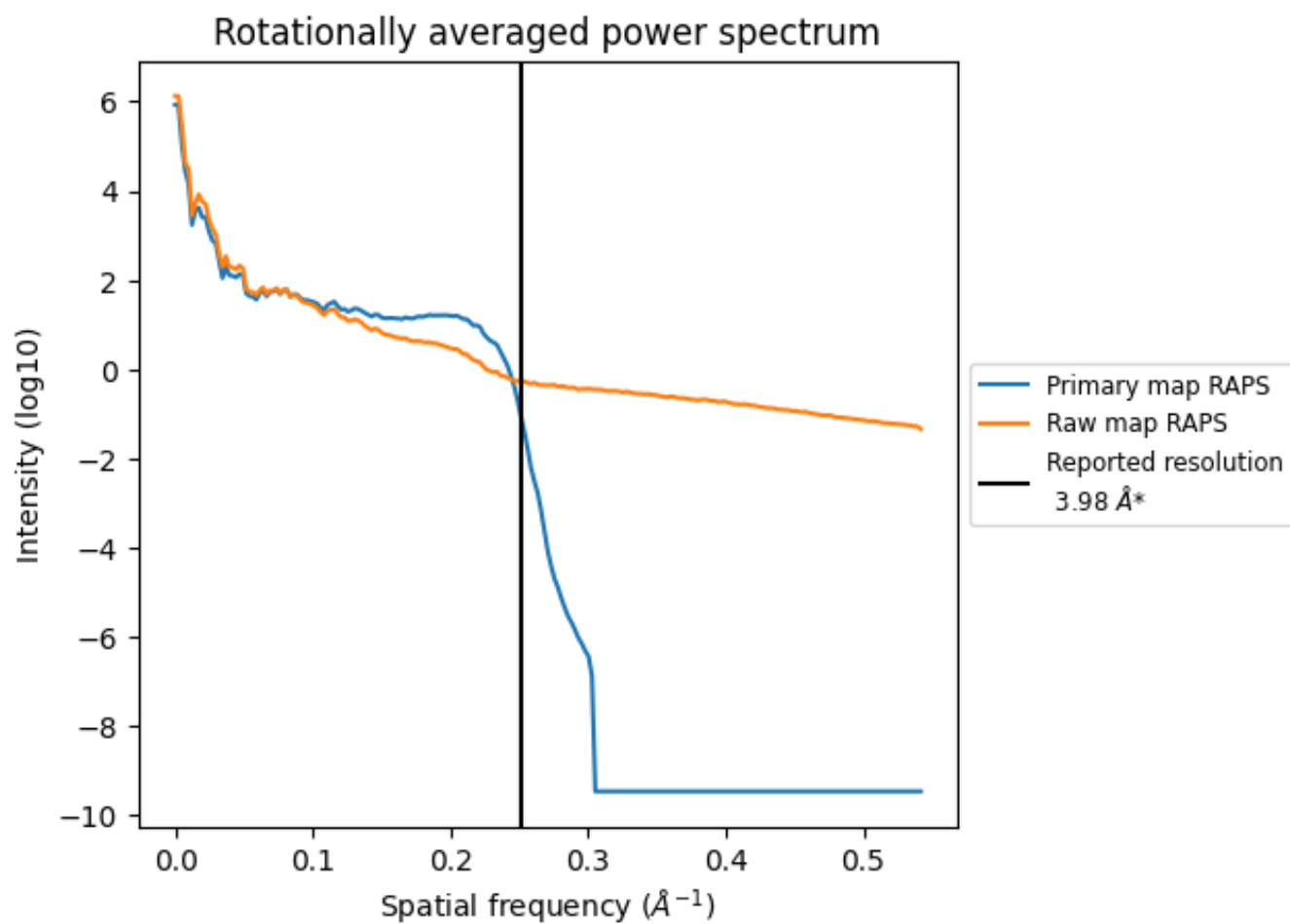
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1715 nm³; this corresponds to an approximate mass of 1550 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

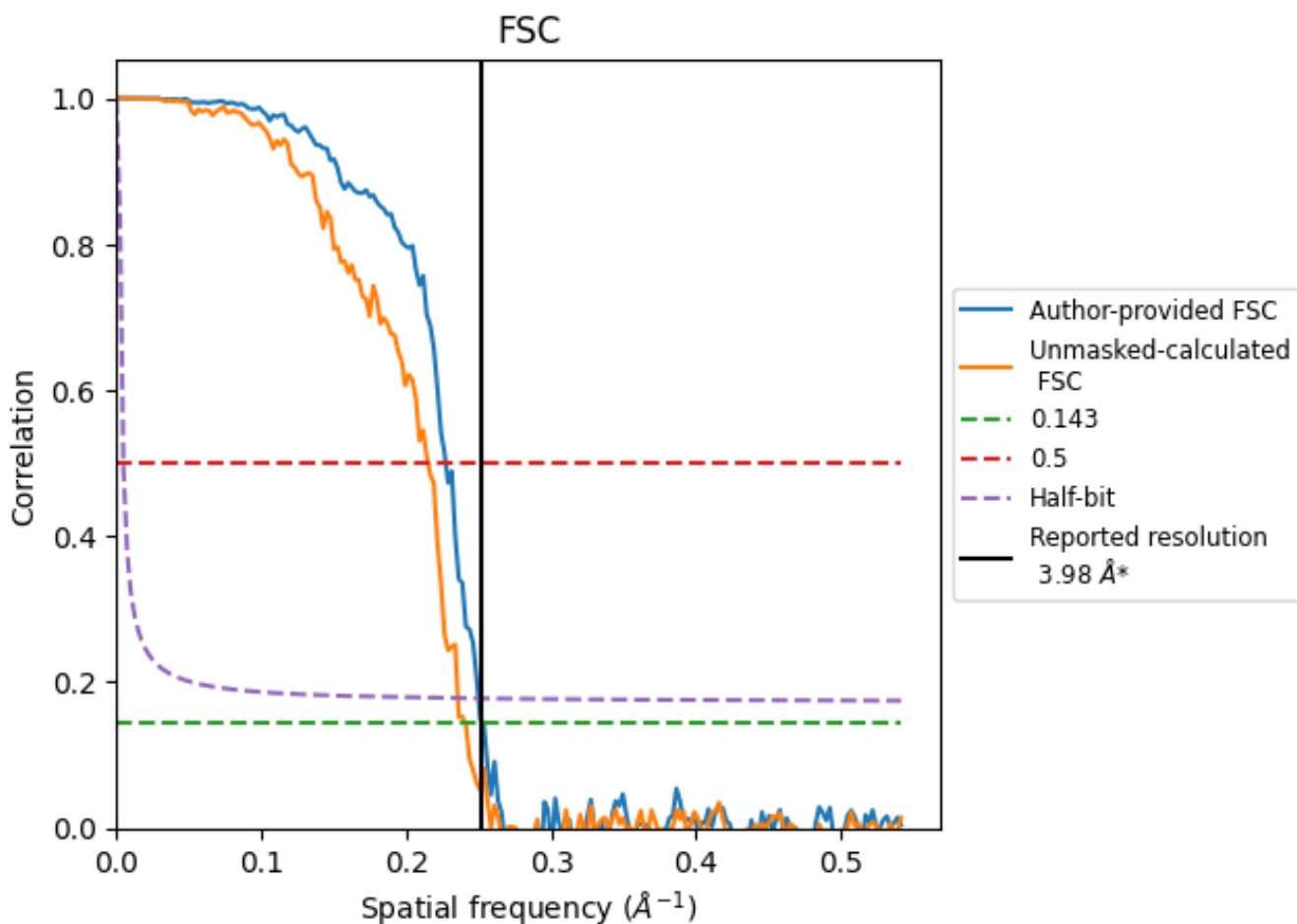


*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.251 Å⁻¹

8.2 Resolution estimates [i](#)

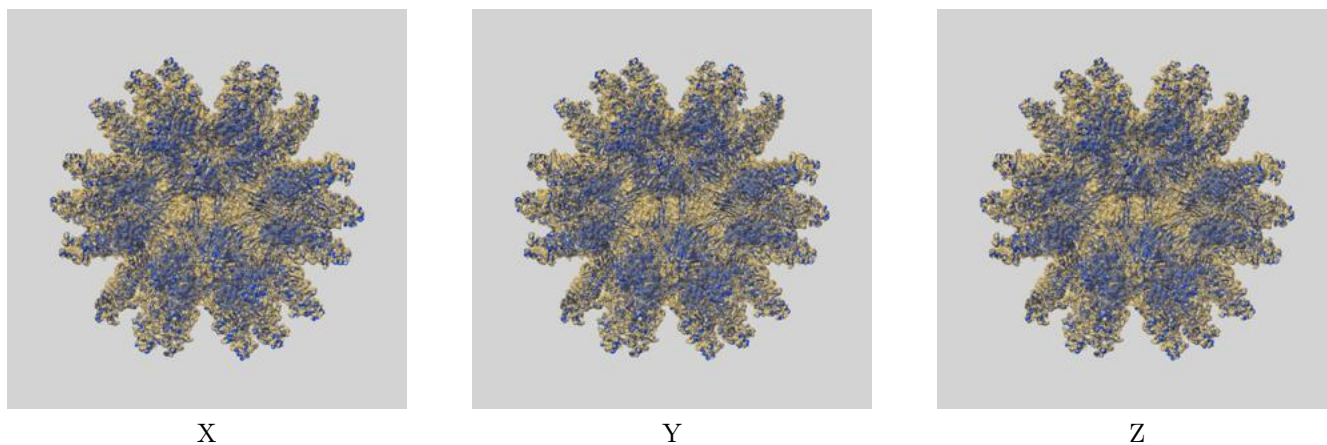
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.98	-	-
Author-provided FSC curve	3.95	4.40	4.00
Unmasked-calculated*	4.15	4.65	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

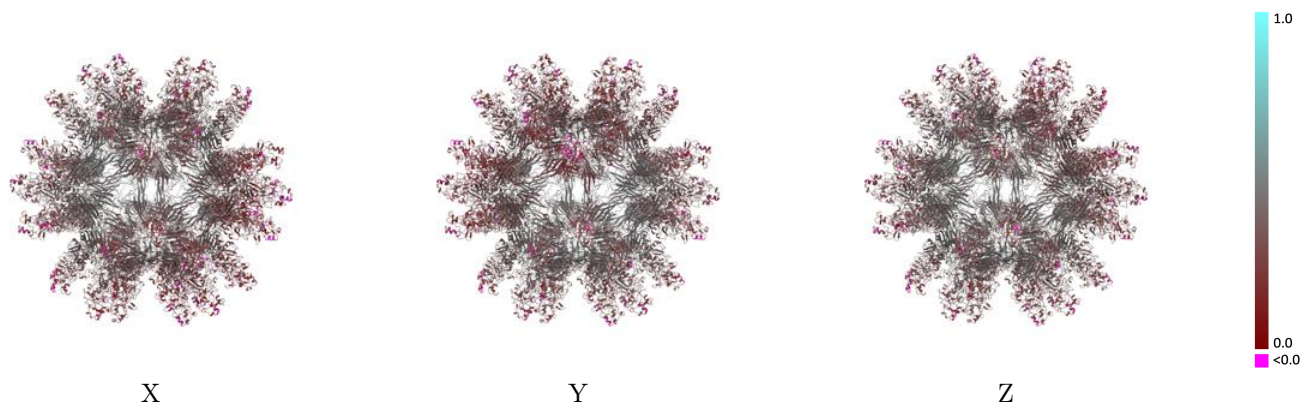
This section contains information regarding the fit between EMDB map EMD-27077 and PDB model 8CYG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



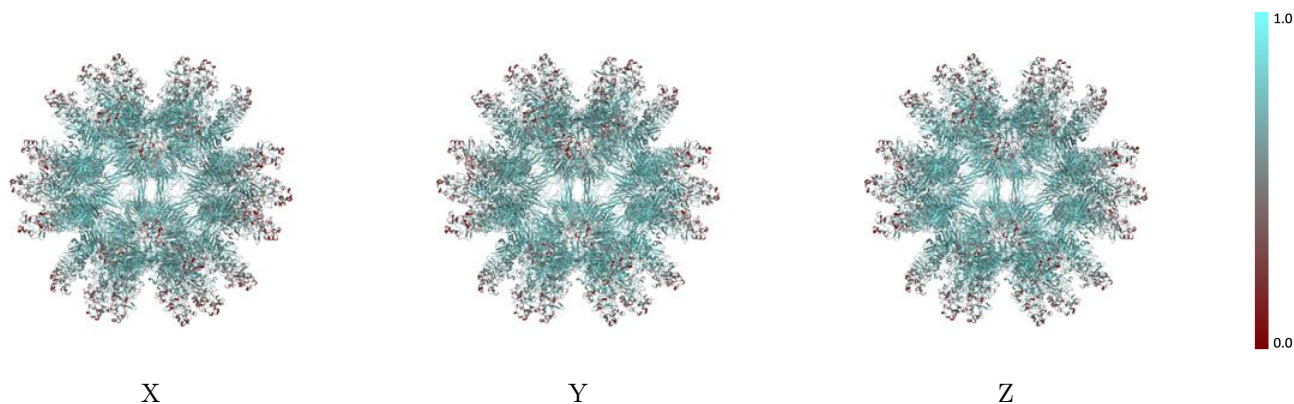
The images above show the 3D surface view of the map at the recommended contour level 2.87 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



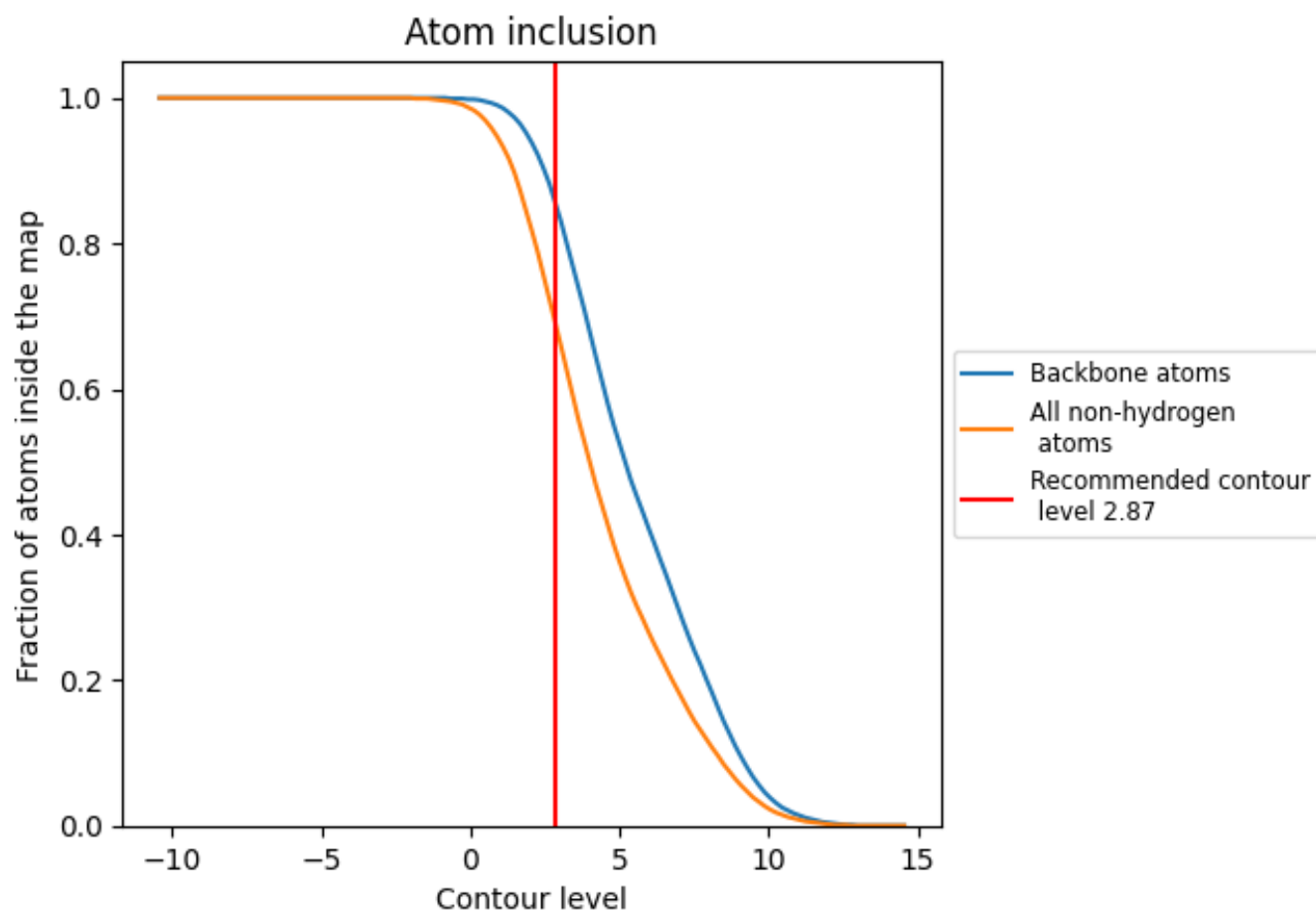
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.87).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 69% 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 (2.87) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.3650
0	 0.7060	 0.3870
1	 0.6280	 0.2950
2	 0.6410	 0.3060
3	 0.7040	 0.3860
4	 0.7080	 0.3860
5	 0.7060	 0.3860
6	 0.7040	 0.3860
7	 0.7050	 0.3870
A	 0.6490	 0.3150
B	 0.6740	 0.3500
C	 0.6740	 0.3520
D	 0.6540	 0.3290
E	 0.6540	 0.3270
F	 0.6820	 0.3570
G	 0.6880	 0.3660
H	 0.6910	 0.3760
I	 0.7040	 0.3880
J	 0.7040	 0.3870
K	 0.7030	 0.3870
L	 0.7010	 0.3860
M	 0.7040	 0.3850
N	 0.6780	 0.3580
O	 0.6120	 0.2580
P	 0.6820	 0.3650
Q	 0.6940	 0.3720
R	 0.6650	 0.3420
S	 0.6680	 0.3380
T	 0.6430	 0.3000
U	 0.6600	 0.3290
V	 0.6410	 0.3010
W	 0.6570	 0.3250
X	 0.6890	 0.3670
Y	 0.6630	 0.3290
Z	 0.6990	 0.3770



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Chain	Atom inclusion	Q-score
a	 0.7060	 0.3900
b	 0.7060	 0.3870
c	 0.7050	 0.3880
d	 0.7040	 0.3860
e	 0.7010	 0.3840
f	 0.7020	 0.3870
g	 0.6970	 0.3820
h	 0.7020	 0.3840
i	 0.7000	 0.3830
j	 0.7060	 0.3820
k	 0.7040	 0.3850
l	 0.7080	 0.3850
m	 0.7050	 0.3880
n	 0.7050	 0.3820
o	 0.7060	 0.3870
p	 0.7030	 0.3880
q	 0.7050	 0.3870
r	 0.7040	 0.3860
s	 0.7050	 0.3850
t	 0.6810	 0.3530
u	 0.7040	 0.3850
v	 0.7050	 0.3880
w	 0.7030	 0.3830
x	 0.7030	 0.3880
y	 0.7020	 0.3840
z	 0.6240	 0.2890