



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 12:58 AM EST

PDB ID : 6E39  
EMDB ID : EMD-8975  
Title : Capsid protein of PCV2 with 2-O-sulfo-alpha-L-idopyranuronic acid and N,O  
6-DISULFO-GLUCOSAMINE  
Authors : Khayat, R.; Dhindwal, S.  
Deposited on : 2018-07-13  
Resolution : 3.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

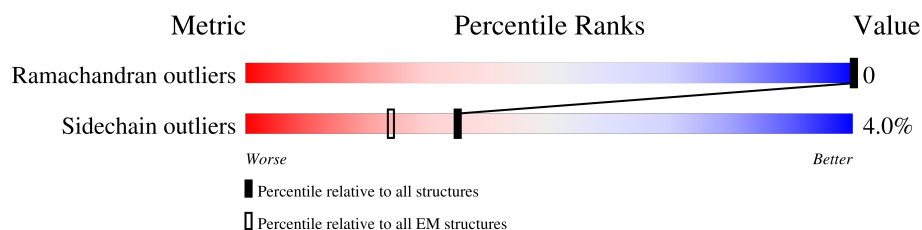
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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













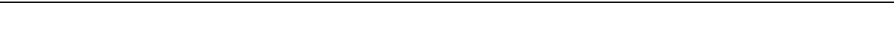

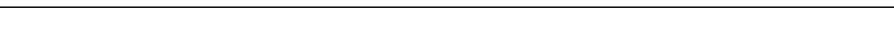
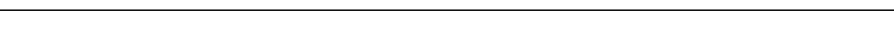











Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A1	233	81% 19%
1	A2	233	78% 19%
1	A3	233	78% 19%
1	A4	233	78% 19%
1	A5	233	78% 19%
1	A6	233	78% 19%
1	A7	233	78% 19%
1	A8	233	78% 19%
1	A9	233	78% 19%











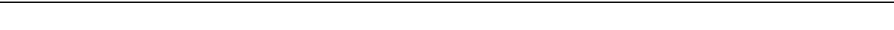

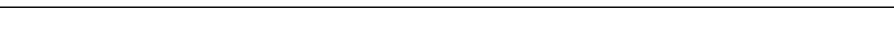
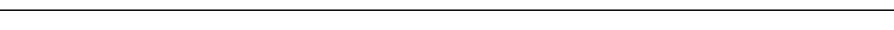











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Mol	Chain	Length	Quality of chain
1	AA	233	 78%19%
1	AB	233	 78%19%
1	AC	233	 78%19%
1	AD	233	 78%19%
1	AE	233	 78%19%
1	AF	233	 78%19%
1	AG	233	 78%19%
1	AH	233	 78%19%
1	AI	233	 78%19%
1	AJ	233	 78%19%
1	AK	233	 78%19%
1	AL	233	 78%19%
1	AM	233	 78%19%
1	AN	233	 78%19%
1	AO	233	 78%19%
1	AP	233	 78%19%
1	AQ	233	 78%19%
1	AR	233	 78%19%
1	AS	233	 78%19%
1	AT	233	 78%19%
1	AU	233	 78%19%
1	AV	233	 78%19%
1	AW	233	 78%19%
1	AX	233	 78%19%
1	AY	233	 78%19%


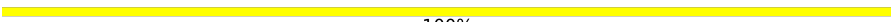
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Mol	Chain	Length	Quality of chain
1	AZ	233	 78%19%
1	Aa	233	 78%19%
1	Ab	233	 78%19%
1	Ac	233	 78%19%
1	Ad	233	 78%19%
1	Ae	233	 78%19%
1	Af	233	 78%19%
1	Ag	233	 78%19%
1	Ah	233	 78%19%
1	Ai	233	 78%19%
1	Aj	233	 78%19%
1	Ak	233	 78%19%
1	Al	233	 78%19%
1	Am	233	 78%19%
1	An	233	 78%19%
1	Ao	233	 78%19%
1	Ap	233	 78%19%
1	Aq	233	 78%19%
1	Ar	233	 78%19%
1	As	233	 78%19%
1	At	233	 78%19%
1	Au	233	 78%19%
1	Av	233	 78%19%
1	Aw	233	 78%19%
1	Ax	233	 78%19%

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Mol	Chain	Length	Quality of chain
1	Ay	233	 78%19%
2	A	2	 100%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 183216 atoms, of which 90180 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 of PCV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A2	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A3	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A4	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A5	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A6	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A7	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A8	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	A9	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AA	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AB	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AC	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AD	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AE	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AF	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AG	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AH	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	AI	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AJ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AK	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AL	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AM	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AN	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AO	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AP	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AQ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AR	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AS	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AT	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AU	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AV	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AW	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AX	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AY	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	AZ	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aa	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ab	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ac	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ad	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ae	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Af	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ag	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ah	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ai	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aj	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ak	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Al	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Am	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	An	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ao	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ap	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aq	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ar	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	As	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	At	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Au	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Av	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Aw	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		
1	Ax	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ay	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

- Molecule 2 is an oligosaccharide called 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid.




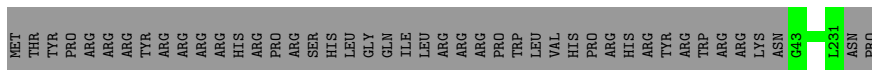
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	2	Total	C	N	O	S	0	0
			36	12	1	20	3		

### 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.

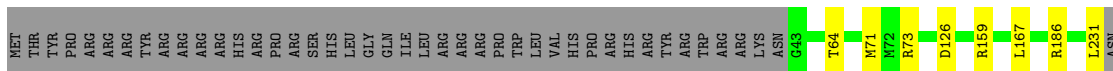
- Molecule 1: Capsid protein of PCV2

Chain A1:  81% 19%




- Molecule 1: Capsid protein of PCV2

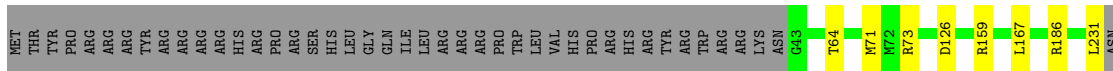
Chain A2:  78% 19%



PRO


- Molecule 1: Capsid protein of PCV2

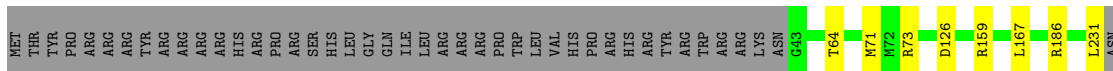
Chain A3:  78% 19%



PRO


- Molecule 1: Capsid protein of PCV2

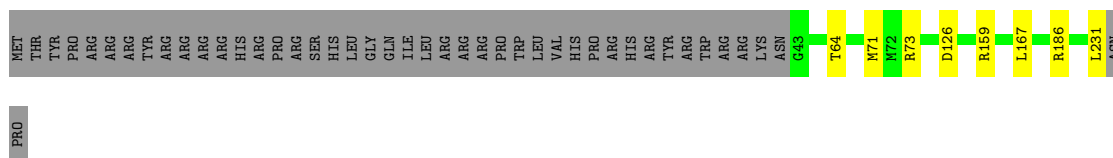
Chain A4:  78% 19%




PRO

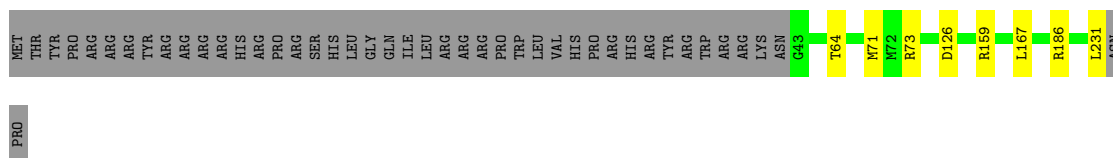
- Molecule 1: Capsid protein of PCV2

Chain A5:  78% 19%




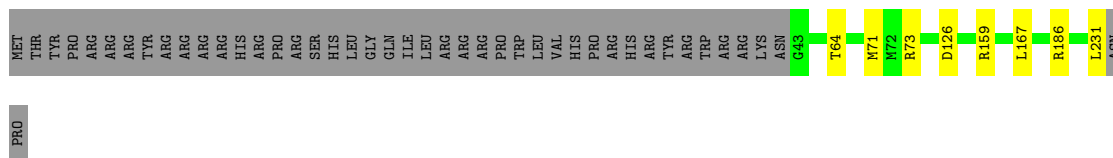
- Molecule 1: Capsid protein of PCV2

Chain A6:  78% 19%




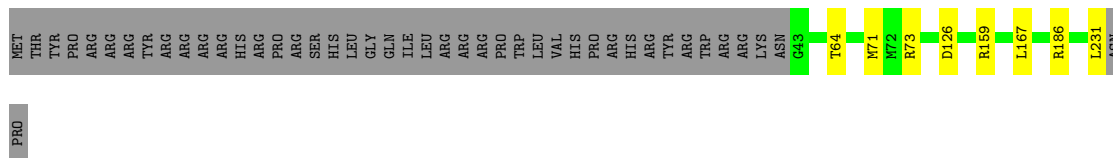
- Molecule 1: Capsid protein of PCV2

Chain A7:  78% 19%




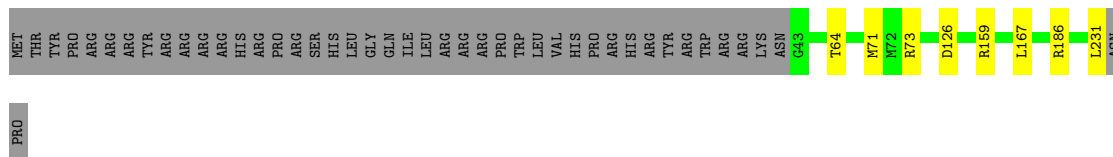
- Molecule 1: Capsid protein of PCV2

Chain A8:  78% 19%




- Molecule 1: Capsid protein of PCV2

Chain A9:  78% 19%




- Molecule 1: Capsid protein of PCV2

Chain AA:  78% 19%



PRO


- Molecule 1: Capsid protein of PCV2

Chain AG:  78% 19%

MET	THR	TYR	PRO	ARG	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	HIS	HIS	ARG	PRO	PRO	SER	SER	HIS	HIS	LEU	GLY	GLN	ILE	LEU	LEU	ARG	ARG	ARG	ARG	PRO	TRP	TRP	VAL	HIS	PRO	ARG	HIS	HIS	ARG	TYR	ARG	TRP	ARG	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN
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PRO


- Molecule 1: Capsid protein of PCV2

Chain AH:  78% 19%

MET	THR	TYR	PRO	ARG	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	HIS	HIS	ARG	PRO	PRO	SER	SER	HIS	HIS	LEU	GLY	GLN	ILE	LEU	LEU	ARG	ARG	ARG	ARG	PRO	TRP	TRP	VAL	HIS	PRO	ARG	HIS	HIS	ARG	TYR	ARG	TRP	ARG	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN
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PRO


- Molecule 1: Capsid protein of PCV2

Chain AI:  78% 19%

MET	THR	TYR	PRO	ARG	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	HIS	HIS	ARG	PRO	PRO	SER	SER	HIS	HIS	LEU	GLY	GLN	ILE	LEU	LEU	ARG	ARG	ARG	ARG	PRO	TRP	TRP	VAL	HIS	PRO	ARG	HIS	HIS	ARG	TYR	ARG	TRP	ARG	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN
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PRO


- Molecule 1: Capsid protein of PCV2

Chain AJ:  78% 19%

MET	THR	TYR	PRO	ARG	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	HIS	HIS	ARG	PRO	PRO	SER	SER	HIS	HIS	LEU	GLY	GLN	ILE	LEU	LEU	ARG	ARG	ARG	ARG	PRO	TRP	TRP	VAL	HIS	PRO	ARG	HIS	HIS	ARG	TYR	ARG	TRP	ARG	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN
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PRO

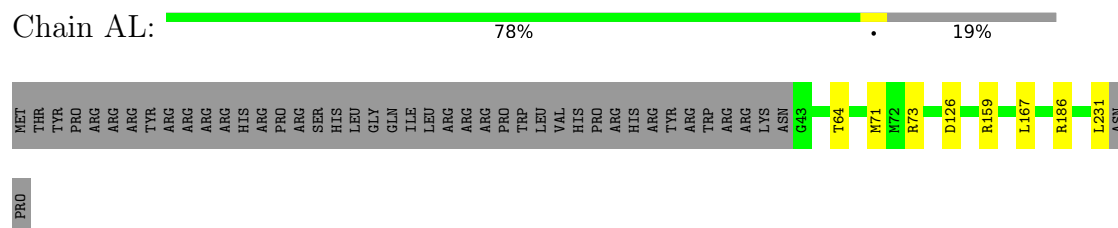
- Molecule 1: Capsid protein of PCV2

Chain AK:  78% 19%

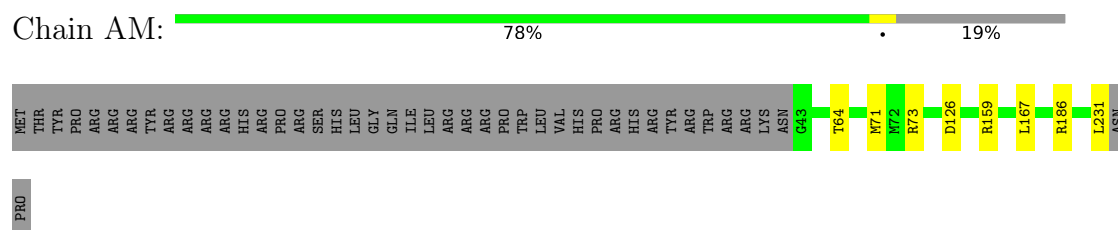
MET	THR	TYR	PRO	ARG	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	HIS	HIS	ARG	PRO	PRO	SER	SER	HIS	HIS	LEU	GLY	GLN	ILE	LEU	LEU	ARG	ARG	ARG	ARG	PRO	TRP	TRP	VAL	HIS	PRO	ARG	HIS	HIS	ARG	TYR	ARG	TRP	ARG	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN
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PRO

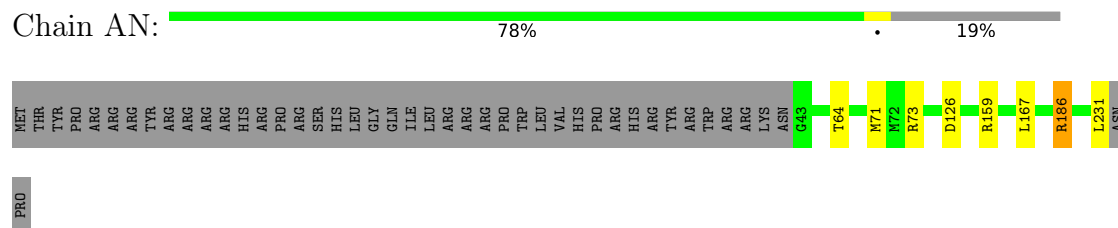
- Molecule 1: Capsid protein of PCV2



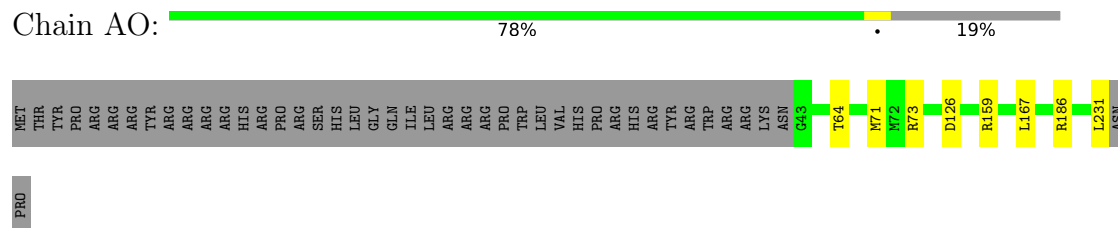
- Molecule 1: Capsid protein of PCV2



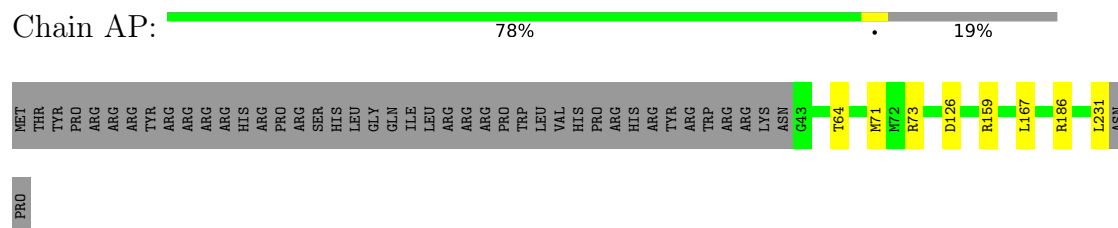
- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2




- Molecule 1: Capsid protein of PCV2



- Molecule 1: Capsid protein of PCV2

MET	TMR	TTR	PRO	ARG	ARG	ARG	ARG	ARG	ARG	HIS	HIS	PRO	PRO	SER	HIS	LEU	GLY	GLN	ILE	LEU	ARG	ARG	ARG	PRO	PRO	TRP	LEU	VAL	HIS	PRO	ARG	ARG	ARG	ARG	TYR	ARG	TRP	ARG	ARG	LYS	LYS	ASN	G43	T64	M71	R73	D126	R159	L167	R186	L231	LSH
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----

PRO

- Chain AR:  78% 19%


MET	THR	TYR	PRO	ARG	ARG	ARG	ARG	ARG	HIS	ARG	PRO	SER	HIS	LEU	GLY	ILE	LEU	ARG	ARG	ARG	PRO	TRP	LEU	VAL	HIS	PRO	ARG	HIS	ARG	TRP	ARG	ARG	LYS	ASN	G43	T64	M71	R72	R73	D126	R159	L167	R186	L231	L231
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

PRO

- Chain AS: 78% 19%

MET	THR	TRP	PRO	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	ARG	SER	HIS	LEU	GLY	GLN	ILE	LEU	ARG	ARG	ARG	PRO	PRO	TRP	LEU	VAL	HIS	PRO	ARG	ARG	HIS	HIS	ARG	ARG	TRP	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	SPV
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----

PRO

- Chain AT:  78% 1% 19%

MET	THR	TRP	PRO	ARG	ARG	TYR	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ASN	G43	T64	M71	M72	M73	D126	R159	L167	R186	L231	L238
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

PRO

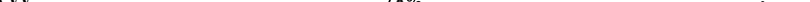
- Chain AU:  78% . 19%

MET	THR	TYR	PRO	ARG	ARG	ARG	ARG	ARG	HIS	HIS	GLY	ILE	LEU	ARG	ARG	ARG	PRO	TRP	LEU	VAL	HIS	PRO	ARG	HIS	ARG	TYR	ARG	TRP	ARG	ARG	LYS	ASN	G43	G44	T64	M71	M72	R73	D126	R159	L167	R186	L231	LSH
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	-----

PRO

- Chain AV:  78% 1% 21%




- Chain AW:  78% 19%



- Chain AX:  78% 19%



- Chain AY:  78% 19%



- Chain AZ:  78% 1% 19%



- Chain Aa:  78% . 19%








- Molecule 1: Capsid protein of PCV2


PRO																																																					
	MET	THR	TYR	PRO	ARG	ARG	TYR	ARG	ARG	ARG	ARG	HIS	PRO	ARG	SER	HIS	LEU	GLY	GLN	ILE	LEU	ARG	ARG	ARG	PRO	PRO	TRP	LEU	VAL	HIS	PRO	PRO	ARG	HIS	ARG	TYR	ARG	TRP	TRP	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231

- Chain Am:  78% • 19%


	PRO																				MET																														
	THR	TYR	PRO	ARG	ARG	TYR	ARG	ARG	ARG	ARG	HIS	ARG	PRO	SER	HIS	LEU	GLY	GLN	ILE	LEU	ARG	ARG	ARG	PRO	TRP	LEU	VAL	HIS	PRO	PRO	ARG	HIS	ARG	TYP	ARG	TRP	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	ASN

- Chain An:  78% 19%


PRO	MET
	THR
	TYR
	PRO
	ARG
	ARG
	TYR
	ARG
	ARG
	ARG
	HIS
	PRO
	ARG
	SER
	HIS
	GLY
	GLN
	ILE
	LEU
	ARG
	ARG
	PRO
	TRP
	LEU
	VAL
	HIS
	PRO
	ARG
	HIS
	ARG
	TYR
	ARG
	TRP
	ARG
	ARG
	LYS
	ASN
	G43
	T64
	M71
	H72
	R73
	D126
	R159
	L167
	R186
	L231
	L581

- Chain Ao:  78% . 19%


PRO	MET
	THR
	TYR
	PRO
	ARG
	ARG
	TYR
	ARG
	ARG
	ARG
	HIS
	PRO
	ARG
	SER
	HIS
	LEU
	GLY
	GLN
	ILE
	LEU
	ARG
	ARG
	PRO
	TRP
	LEU
	VAL
	HIS
	PRO
	ARG
	HIS
	ARG
	TYR
	TRP
	ARG
	ARG
	LYS
	ASN
	G43
	T64
	M71
	H72
	R73
	D126
	R159
	L167
	R186
	L231
	L581

- Chain Ap:  78% . 19%

PRO	MET																																																	
	THR	TYR	PRO	ARG	ARG	TYR	ARG	ARG	ARG	ARG	HIS	ARG	PRO	ARG	SER	HIS	LEU	GLN	ILE	LEU	ARG	ARG	ARG	PRO	TRP	LEU	VAL	HIS	PRO	ARG	HIS	ARG	TYR	ARG	TRP	ARG	ARG	LYS	ASN	G43	T64	M71	M72	R73	D126	R159	L167	R186	L231	L231

- Chain Aq:  78% 19%



- Chain Ar:  78% • 19%

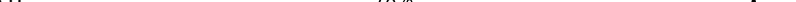


- Chain As:  78% • 19%




- Chain At: 78% 19%



- Chain Au:  78% 19%

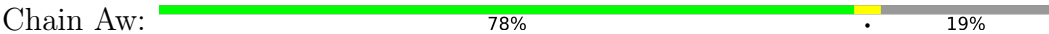


- Chain Av:  78% . 19%



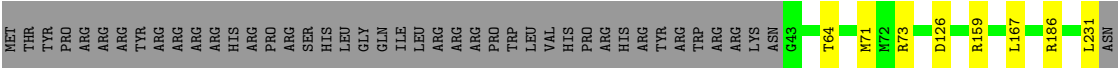
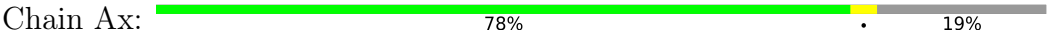
PRO

• Molecule 1: Capsid protein of PCV2



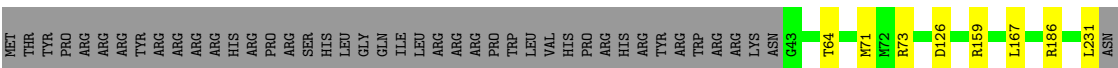
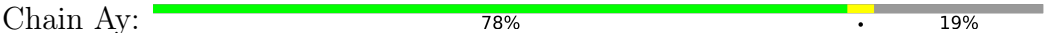
PRO

• Molecule 1: Capsid protein of PCV2



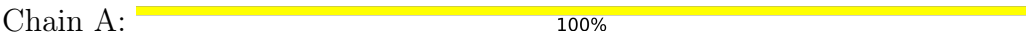
PRO

• Molecule 1: Capsid protein of PCV2



PRO

• Molecule 2: 2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid



IDS1  
SGN2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	66701	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Per particle estimation	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	32	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	0.079	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	327.0, 327.0, 327.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A1	0.41	0/1597	0.56	0/2175
1	A2	0.76	0/1597	0.63	1/2175 (0.0%)
1	A3	0.76	0/1597	0.63	1/2175 (0.0%)
1	A4	0.76	0/1597	0.63	1/2175 (0.0%)
1	A5	0.76	0/1597	0.63	1/2175 (0.0%)
1	A6	0.76	0/1597	0.63	1/2175 (0.0%)
1	A7	0.76	0/1597	0.63	1/2175 (0.0%)
1	A8	0.76	0/1597	0.63	1/2175 (0.0%)
1	A9	0.76	0/1597	0.63	1/2175 (0.0%)
1	AA	0.76	0/1597	0.63	1/2175 (0.0%)
1	AB	0.76	0/1597	0.63	1/2175 (0.0%)
1	AC	0.76	0/1597	0.63	1/2175 (0.0%)
1	AD	0.76	0/1597	0.63	1/2175 (0.0%)
1	AE	0.76	0/1597	0.63	1/2175 (0.0%)
1	AF	0.76	0/1597	0.63	1/2175 (0.0%)
1	AG	0.76	0/1597	0.63	1/2175 (0.0%)
1	AH	0.76	0/1597	0.63	1/2175 (0.0%)
1	AI	0.76	0/1597	0.63	1/2175 (0.0%)
1	AJ	0.76	0/1597	0.63	1/2175 (0.0%)
1	AK	0.76	0/1597	0.63	1/2175 (0.0%)
1	AL	0.76	0/1597	0.63	1/2175 (0.0%)
1	AM	0.76	0/1597	0.63	1/2175 (0.0%)
1	AN	0.76	0/1597	0.63	1/2175 (0.0%)
1	AO	0.76	0/1597	0.63	1/2175 (0.0%)
1	AP	0.76	0/1597	0.63	1/2175 (0.0%)
1	AQ	0.76	0/1597	0.63	1/2175 (0.0%)
1	AR	0.76	0/1597	0.63	1/2175 (0.0%)
1	AS	0.76	0/1597	0.63	1/2175 (0.0%)
1	AT	0.76	0/1597	0.63	1/2175 (0.0%)
1	AU	0.76	0/1597	0.63	1/2175 (0.0%)
1	AV	0.76	0/1597	0.63	1/2175 (0.0%)
1	AW	0.76	0/1597	0.63	1/2175 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AX	0.76	0/1597	0.63	1/2175 (0.0%)
1	AY	0.76	0/1597	0.63	1/2175 (0.0%)
1	AZ	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aa	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ab	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ac	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ad	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ae	0.76	0/1597	0.63	1/2175 (0.0%)
1	Af	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ag	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ah	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ai	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aj	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ak	0.76	0/1597	0.63	1/2175 (0.0%)
1	Al	0.76	0/1597	0.63	1/2175 (0.0%)
1	Am	0.76	0/1597	0.63	1/2175 (0.0%)
1	An	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ao	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ap	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aq	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ar	0.76	0/1597	0.63	1/2175 (0.0%)
1	As	0.76	0/1597	0.63	1/2175 (0.0%)
1	At	0.76	0/1597	0.63	1/2175 (0.0%)
1	Au	0.76	0/1597	0.63	1/2175 (0.0%)
1	Av	0.76	0/1597	0.63	1/2175 (0.0%)
1	Aw	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ax	0.76	0/1597	0.63	1/2175 (0.0%)
1	Ay	0.76	0/1597	0.63	1/2175 (0.0%)
All	All	0.76	0/95820	0.63	59/130500 (0.0%)

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	AN	0	1

There are no bond length outliers.

All (59) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AD	159	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	AI	159	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	AV	159	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	A3	159	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	Ak	159	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	AF	159	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	Ag	159	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	AS	159	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	Ap	159	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A7	159	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	Af	159	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	AX	159	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	Am	159	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	AM	159	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	Ah	159	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	Aw	159	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	AU	159	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	AT	159	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A9	159	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	Ae	159	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	Ao	159	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	AO	159	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	Aj	159	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	Ai	159	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	At	159	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	Ac	159	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A5	159	ARG	NE-CZ-NH2	5.99	123.29	120.30
1	Ar	159	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	AQ	159	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	AR	159	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	Aa	159	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	Ab	159	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	AJ	159	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A4	159	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	AZ	159	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	AE	159	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	AN	159	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	AW	159	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	AG	159	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	AK	159	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	An	159	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	AL	159	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	A2	159	ARG	NE-CZ-NH2	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AP	159	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	As	159	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	AA	159	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	AH	159	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	Ad	159	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	Ay	159	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	Au	159	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	Av	159	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	AY	159	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	AB	159	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	AC	159	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A8	159	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	Al	159	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	Ax	159	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	A6	159	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	Aq	159	ARG	NE-CZ-NH2	5.72	123.16	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AN	186	ARG	Sidechain

## 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	A1	187/233 (80%)	178 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A2	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A3	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A4	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A5	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A6	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A7	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	A8	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	A9	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AA	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AB	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AC	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AD	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AE	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AF	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AG	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AH	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AI	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AJ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AK	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AL	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AM	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AN	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AO	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AP	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AQ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AR	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AS	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	AT	187/233 (80%)	179 (96%)	8 (4%)	0	100	100
1	AU	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AV	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AW	187/233 (80%)	181 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AY	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	AZ	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Aa	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ab	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ac	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ad	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ae	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Af	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ag	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ah	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ai	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Aj	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Ak	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Al	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Am	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	An	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ao	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ap	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	Aq	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ar	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	As	187/233 (80%)	180 (96%)	7 (4%)	0	100	100
1	At	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Au	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Av	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Aw	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ax	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
1	Ay	187/233 (80%)	181 (97%)	6 (3%)	0	100	100
All	All	11220/13980 (80%)	10839 (97%)	381 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	172/215 (80%)	172 (100%)	0	100	100
1	A2	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A3	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A4	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A5	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A6	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A7	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A8	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	A9	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AA	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AB	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AC	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AD	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AE	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AF	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AG	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AH	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AI	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AJ	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AK	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AL	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AM	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AN	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AO	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AP	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AQ	172/215 (80%)	165 (96%)	7 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AS	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AT	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AU	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AV	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AW	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AX	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AY	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	AZ	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Aa	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ab	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ac	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ad	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ae	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Af	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ag	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ah	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ai	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Aj	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ak	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Al	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Am	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	An	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ao	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ap	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Aq	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ar	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	As	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	At	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Au	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Av	172/215 (80%)	165 (96%)	7 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aw	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ax	172/215 (80%)	165 (96%)	7 (4%)	30	63
1	Ay	172/215 (80%)	165 (96%)	7 (4%)	30	63
All	All	10320/12900 (80%)	9907 (96%)	413 (4%)	35	64

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A2	64	THR
1	A2	71	MET
1	A2	73	ARG
1	A2	126	ASP
1	A2	167	LEU
1	A2	186	ARG
1	A2	231	LEU
1	A3	64	THR
1	A3	71	MET
1	A3	73	ARG
1	A3	126	ASP
1	A3	167	LEU
1	A3	186	ARG
1	A3	231	LEU
1	A4	64	THR
1	A4	71	MET
1	A4	73	ARG
1	A4	126	ASP
1	A4	167	LEU
1	A4	186	ARG
1	A4	231	LEU
1	A5	64	THR
1	A5	71	MET
1	A5	73	ARG
1	A5	126	ASP
1	A5	167	LEU
1	A5	186	ARG
1	A5	231	LEU
1	A6	64	THR
1	A6	71	MET
1	A6	73	ARG
1	A6	126	ASP
1	A6	167	LEU

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Mol	Chain	Res	Type
1	A6	186	ARG
1	A6	231	LEU
1	A7	64	THR
1	A7	71	MET
1	A7	73	ARG
1	A7	126	ASP
1	A7	167	LEU
1	A7	186	ARG
1	A7	231	LEU
1	A8	64	THR
1	A8	71	MET
1	A8	73	ARG
1	A8	126	ASP
1	A8	167	LEU
1	A8	186	ARG
1	A8	231	LEU
1	A9	64	THR
1	A9	71	MET
1	A9	73	ARG
1	A9	126	ASP
1	A9	167	LEU
1	A9	186	ARG
1	A9	231	LEU
1	AA	64	THR
1	AA	71	MET
1	AA	73	ARG
1	AA	126	ASP
1	AA	167	LEU
1	AA	186	ARG
1	AA	231	LEU
1	AB	64	THR
1	AB	71	MET
1	AB	73	ARG
1	AB	126	ASP
1	AB	167	LEU
1	AB	186	ARG
1	AB	231	LEU
1	AC	64	THR
1	AC	71	MET
1	AC	73	ARG
1	AC	126	ASP
1	AC	167	LEU

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Mol	Chain	Res	Type
1	AC	186	ARG
1	AC	231	LEU
1	AD	64	THR
1	AD	71	MET
1	AD	73	ARG
1	AD	126	ASP
1	AD	167	LEU
1	AD	186	ARG
1	AD	231	LEU
1	AE	64	THR
1	AE	71	MET
1	AE	73	ARG
1	AE	126	ASP
1	AE	167	LEU
1	AE	186	ARG
1	AE	231	LEU
1	AF	64	THR
1	AF	71	MET
1	AF	73	ARG
1	AF	126	ASP
1	AF	167	LEU
1	AF	186	ARG
1	AF	231	LEU
1	AG	64	THR
1	AG	71	MET
1	AG	73	ARG
1	AG	126	ASP
1	AG	167	LEU
1	AG	186	ARG
1	AG	231	LEU
1	AH	64	THR
1	AH	71	MET
1	AH	73	ARG
1	AH	126	ASP
1	AH	167	LEU
1	AH	186	ARG
1	AH	231	LEU
1	AI	64	THR
1	AI	71	MET
1	AI	73	ARG
1	AI	126	ASP
1	AI	167	LEU

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Mol	Chain	Res	Type
1	AI	186	ARG
1	AI	231	LEU
1	AJ	64	THR
1	AJ	71	MET
1	AJ	73	ARG
1	AJ	126	ASP
1	AJ	167	LEU
1	AJ	186	ARG
1	AJ	231	LEU
1	AK	64	THR
1	AK	71	MET
1	AK	73	ARG
1	AK	126	ASP
1	AK	167	LEU
1	AK	186	ARG
1	AK	231	LEU
1	AL	64	THR
1	AL	71	MET
1	AL	73	ARG
1	AL	126	ASP
1	AL	167	LEU
1	AL	186	ARG
1	AL	231	LEU
1	AM	64	THR
1	AM	71	MET
1	AM	73	ARG
1	AM	126	ASP
1	AM	167	LEU
1	AM	186	ARG
1	AM	231	LEU
1	AN	64	THR
1	AN	71	MET
1	AN	73	ARG
1	AN	126	ASP
1	AN	167	LEU
1	AN	186	ARG
1	AN	231	LEU
1	AO	64	THR
1	AO	71	MET
1	AO	73	ARG
1	AO	126	ASP
1	AO	167	LEU

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Mol	Chain	Res	Type
1	AO	186	ARG
1	AO	231	LEU
1	AP	64	THR
1	AP	71	MET
1	AP	73	ARG
1	AP	126	ASP
1	AP	167	LEU
1	AP	186	ARG
1	AP	231	LEU
1	AQ	64	THR
1	AQ	71	MET
1	AQ	73	ARG
1	AQ	126	ASP
1	AQ	167	LEU
1	AQ	186	ARG
1	AQ	231	LEU
1	AR	64	THR
1	AR	71	MET
1	AR	73	ARG
1	AR	126	ASP
1	AR	167	LEU
1	AR	186	ARG
1	AR	231	LEU
1	AS	64	THR
1	AS	71	MET
1	AS	73	ARG
1	AS	126	ASP
1	AS	167	LEU
1	AS	186	ARG
1	AS	231	LEU
1	AT	64	THR
1	AT	71	MET
1	AT	73	ARG
1	AT	126	ASP
1	AT	167	LEU
1	AT	186	ARG
1	AT	231	LEU
1	AU	64	THR
1	AU	71	MET
1	AU	73	ARG
1	AU	126	ASP
1	AU	167	LEU

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Mol	Chain	Res	Type
1	AU	186	ARG
1	AU	231	LEU
1	AV	64	THR
1	AV	71	MET
1	AV	73	ARG
1	AV	126	ASP
1	AV	167	LEU
1	AV	186	ARG
1	AV	231	LEU
1	AW	64	THR
1	AW	71	MET
1	AW	73	ARG
1	AW	126	ASP
1	AW	167	LEU
1	AW	186	ARG
1	AW	231	LEU
1	AX	64	THR
1	AX	71	MET
1	AX	73	ARG
1	AX	126	ASP
1	AX	167	LEU
1	AX	186	ARG
1	AX	231	LEU
1	AY	64	THR
1	AY	71	MET
1	AY	73	ARG
1	AY	126	ASP
1	AY	167	LEU
1	AY	186	ARG
1	AY	231	LEU
1	AZ	64	THR
1	AZ	71	MET
1	AZ	73	ARG
1	AZ	126	ASP
1	AZ	167	LEU
1	AZ	186	ARG
1	AZ	231	LEU
1	Aa	64	THR
1	Aa	71	MET
1	Aa	73	ARG
1	Aa	126	ASP
1	Aa	167	LEU

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Mol	Chain	Res	Type
1	Aa	186	ARG
1	Aa	231	LEU
1	Ab	64	THR
1	Ab	71	MET
1	Ab	73	ARG
1	Ab	126	ASP
1	Ab	167	LEU
1	Ab	186	ARG
1	Ab	231	LEU
1	Ac	64	THR
1	Ac	71	MET
1	Ac	73	ARG
1	Ac	126	ASP
1	Ac	167	LEU
1	Ac	186	ARG
1	Ac	231	LEU
1	Ad	64	THR
1	Ad	71	MET
1	Ad	73	ARG
1	Ad	126	ASP
1	Ad	167	LEU
1	Ad	186	ARG
1	Ad	231	LEU
1	Ae	64	THR
1	Ae	71	MET
1	Ae	73	ARG
1	Ae	126	ASP
1	Ae	167	LEU
1	Ae	186	ARG
1	Ae	231	LEU
1	Af	64	THR
1	Af	71	MET
1	Af	73	ARG
1	Af	126	ASP
1	Af	167	LEU
1	Af	186	ARG
1	Af	231	LEU
1	Ag	64	THR
1	Ag	71	MET
1	Ag	73	ARG
1	Ag	126	ASP
1	Ag	167	LEU

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Mol	Chain	Res	Type
1	Ag	186	ARG
1	Ag	231	LEU
1	Ah	64	THR
1	Ah	71	MET
1	Ah	73	ARG
1	Ah	126	ASP
1	Ah	167	LEU
1	Ah	186	ARG
1	Ah	231	LEU
1	Ai	64	THR
1	Ai	71	MET
1	Ai	73	ARG
1	Ai	126	ASP
1	Ai	167	LEU
1	Ai	186	ARG
1	Ai	231	LEU
1	Aj	64	THR
1	Aj	71	MET
1	Aj	73	ARG
1	Aj	126	ASP
1	Aj	167	LEU
1	Aj	186	ARG
1	Aj	231	LEU
1	Ak	64	THR
1	Ak	71	MET
1	Ak	73	ARG
1	Ak	126	ASP
1	Ak	167	LEU
1	Ak	186	ARG
1	Ak	231	LEU
1	Al	64	THR
1	Al	71	MET
1	Al	73	ARG
1	Al	126	ASP
1	Al	167	LEU
1	Al	186	ARG
1	Al	231	LEU
1	Am	64	THR
1	Am	71	MET
1	Am	73	ARG
1	Am	126	ASP
1	Am	167	LEU

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Mol	Chain	Res	Type
1	Am	186	ARG
1	Am	231	LEU
1	An	64	THR
1	An	71	MET
1	An	73	ARG
1	An	126	ASP
1	An	167	LEU
1	An	186	ARG
1	An	231	LEU
1	Ao	64	THR
1	Ao	71	MET
1	Ao	73	ARG
1	Ao	126	ASP
1	Ao	167	LEU
1	Ao	186	ARG
1	Ao	231	LEU
1	Ap	64	THR
1	Ap	71	MET
1	Ap	73	ARG
1	Ap	126	ASP
1	Ap	167	LEU
1	Ap	186	ARG
1	Ap	231	LEU
1	Aq	64	THR
1	Aq	71	MET
1	Aq	73	ARG
1	Aq	126	ASP
1	Aq	167	LEU
1	Aq	186	ARG
1	Aq	231	LEU
1	Ar	64	THR
1	Ar	71	MET
1	Ar	73	ARG
1	Ar	126	ASP
1	Ar	167	LEU
1	Ar	186	ARG
1	Ar	231	LEU
1	As	64	THR
1	As	71	MET
1	As	73	ARG
1	As	126	ASP
1	As	167	LEU

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Mol	Chain	Res	Type
1	As	186	ARG
1	As	231	LEU
1	At	64	THR
1	At	71	MET
1	At	73	ARG
1	At	126	ASP
1	At	167	LEU
1	At	186	ARG
1	At	231	LEU
1	Au	64	THR
1	Au	71	MET
1	Au	73	ARG
1	Au	126	ASP
1	Au	167	LEU
1	Au	186	ARG
1	Au	231	LEU
1	Av	64	THR
1	Av	71	MET
1	Av	73	ARG
1	Av	126	ASP
1	Av	167	LEU
1	Av	186	ARG
1	Av	231	LEU
1	Aw	64	THR
1	Aw	71	MET
1	Aw	73	ARG
1	Aw	126	ASP
1	Aw	167	LEU
1	Aw	186	ARG
1	Aw	231	LEU
1	Ax	64	THR
1	Ax	71	MET
1	Ax	73	ARG
1	Ax	126	ASP
1	Ax	167	LEU
1	Ax	186	ARG
1	Ax	231	LEU
1	Ay	64	THR
1	Ay	71	MET
1	Ay	73	ARG
1	Ay	126	ASP
1	Ay	167	LEU

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Mol	Chain	Res	Type
1	Ay	186	ARG
1	Ay	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	148	HIS
1	A1	152	GLN
1	A1	178	ASN
1	A1	181	ASN
1	A1	195	HIS
1	A1	212	ASN
1	A2	212	ASN
1	A3	212	ASN
1	A4	212	ASN
1	A5	128	ASN
1	A5	212	ASN
1	A6	212	ASN
1	A7	212	ASN
1	A8	128	ASN
1	A8	212	ASN
1	A9	212	ASN
1	AA	128	ASN
1	AA	212	ASN
1	AB	212	ASN
1	AC	212	ASN
1	AD	212	ASN
1	AE	212	ASN
1	AF	212	ASN
1	AG	128	ASN
1	AG	212	ASN
1	AH	212	ASN
1	AI	128	ASN
1	AI	212	ASN
1	AJ	128	ASN
1	AJ	212	ASN
1	AK	212	ASN
1	AL	128	ASN
1	AL	212	ASN
1	AM	212	ASN
1	AN	212	ASN
1	AO	212	ASN

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Mol	Chain	Res	Type
1	AP	212	ASN
1	AQ	212	ASN
1	AR	212	ASN
1	AS	128	ASN
1	AS	212	ASN
1	AT	212	ASN
1	AU	212	ASN
1	AV	212	ASN
1	AW	212	ASN
1	AX	212	ASN
1	AY	212	ASN
1	AZ	212	ASN
1	Aa	212	ASN
1	Ab	212	ASN
1	Ac	212	ASN
1	Ad	212	ASN
1	Ae	212	ASN
1	Af	212	ASN
1	Ag	212	ASN
1	Ah	128	ASN
1	Ah	212	ASN
1	Ai	212	ASN
1	Aj	128	ASN
1	Aj	212	ASN
1	Ak	212	ASN
1	Al	212	ASN
1	Am	128	ASN
1	Am	212	ASN
1	An	212	ASN
1	Ao	212	ASN
1	Ap	128	ASN
1	Ap	212	ASN
1	Aq	212	ASN
1	Ar	212	ASN
1	As	212	ASN
1	At	212	ASN
1	Au	128	ASN
1	Au	212	ASN
1	Av	212	ASN
1	Aw	128	ASN
1	Aw	212	ASN
1	Ax	212	ASN

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Mol	Chain	Res	Type
1	Ay	212	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

2 monosaccharides 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
2	IDS	A	1	2	17,17,17	1.15	2 (11%)	20,26,26	1.58	2 (10%)
2	SGN	A	2	2	18,19,20	1.25	2 (11%)	22,29,31	1.44	4 (18%)

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
2	IDS	A	1	2	-	7/9/29/29	0/1/1/1
2	SGN	A	2	2	-	3/11/28/31	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	SGN	S1-N2	3.29	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	IDS	O6B-C6	-2.88	1.21	1.30
2	A	1	IDS	O2-C2	-2.28	1.41	1.46
2	A	2	SGN	O5-C1	-2.23	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	IDS	C2-O2-S	4.91	128.36	118.88
2	A	2	SGN	O1S-S1-O2S	-3.31	112.34	120.16
2	A	2	SGN	O4-C4-C5	-2.95	101.97	109.30
2	A	1	IDS	O6B-C6-O6A	-2.72	117.91	124.09
2	A	2	SGN	O1S-S1-N2	-2.34	104.61	108.87
2	A	2	SGN	O4-C4-C3	2.28	115.61	110.35

There are no chirality outliers.

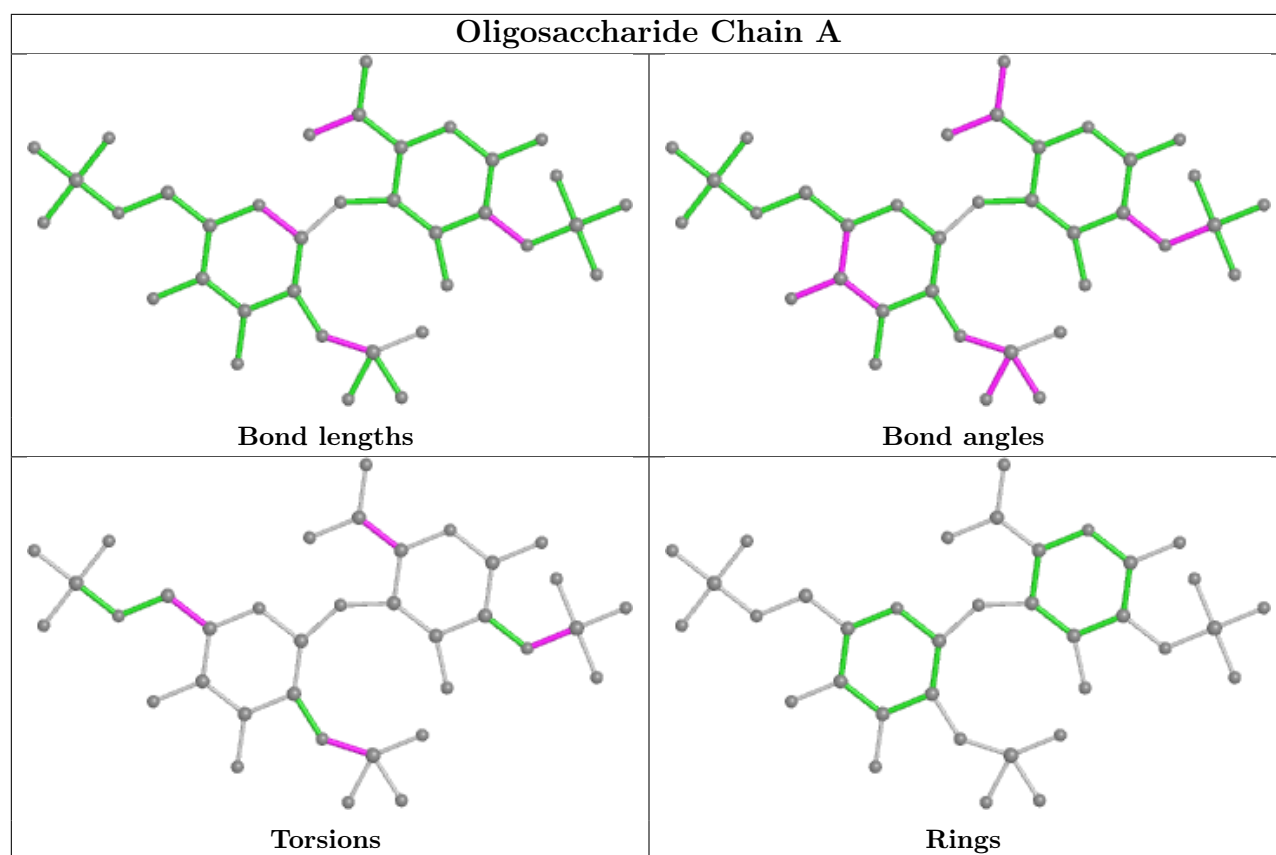
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	IDS	C4-C5-C6-O6A
2	A	1	IDS	C4-C5-C6-O6B
2	A	1	IDS	C2-O2-S-O3S
2	A	2	SGN	C4-C5-C6-O6
2	A	2	SGN	O5-C5-C6-O6
2	A	1	IDS	C2-O2-S-O1S
2	A	1	IDS	C2-O2-S-O2S
2	A	2	SGN	C2-N2-S1-O2S
2	A	1	IDS	O5-C5-C6-O6A
2	A	1	IDS	O5-C5-C6-O6B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

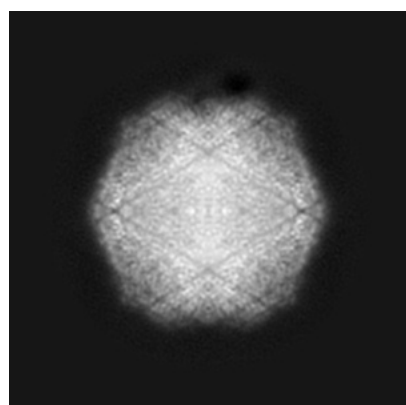
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8975. These allow visual inspection of the internal detail of the map and identification of artifacts.

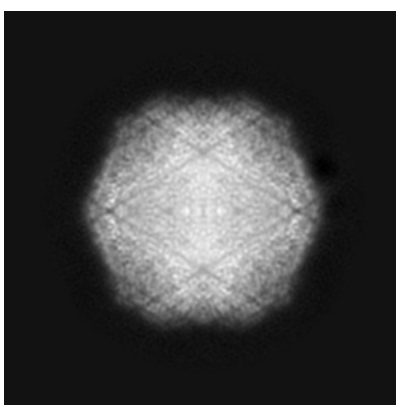
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

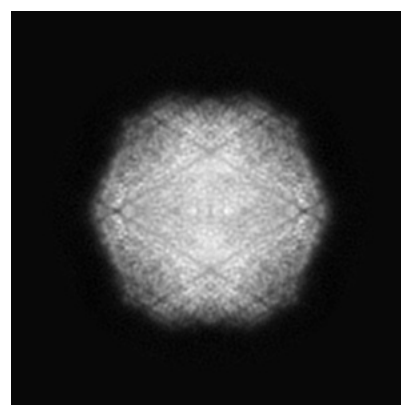
#### 6.1.1 Primary map



X



Y

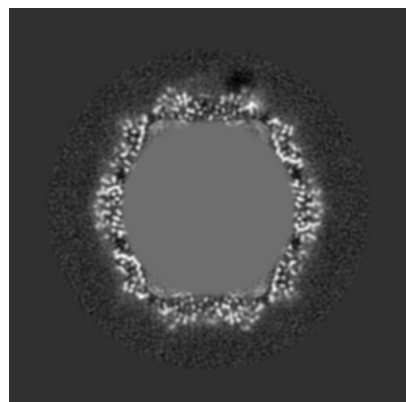


Z

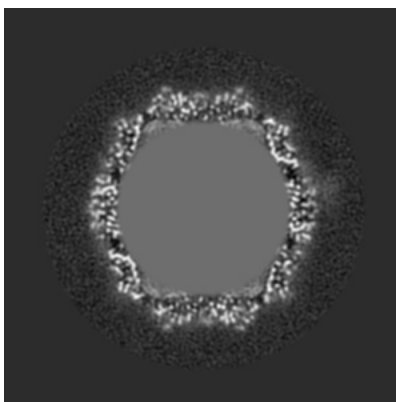
The images above show the map projected in three orthogonal directions.

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

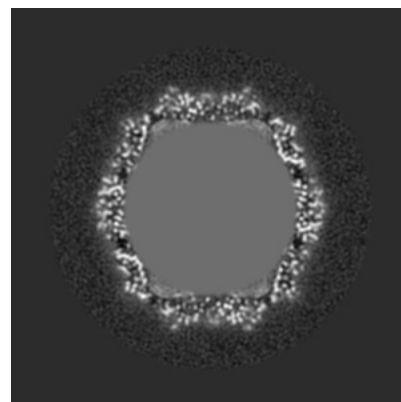
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

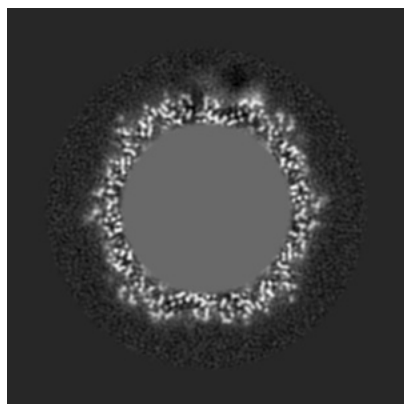


Z Index: 150

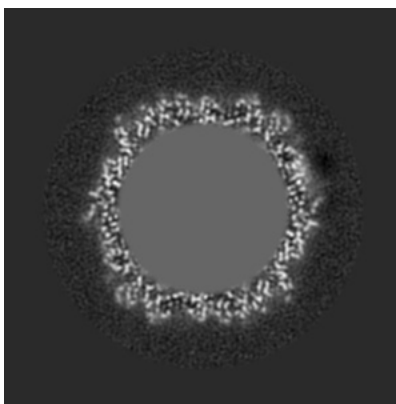
The images above show central slices of the map in three orthogonal directions.

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

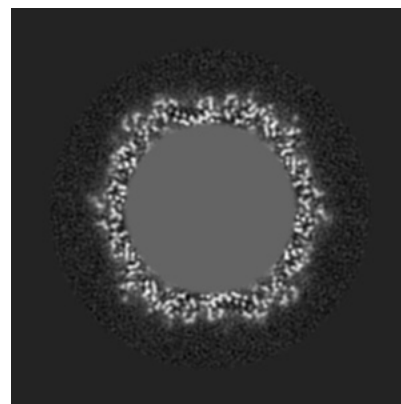
### 6.3.1 Primary map



X Index: 161



Y Index: 162



Z Index: 137

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

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

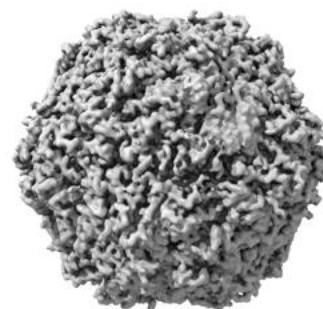
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

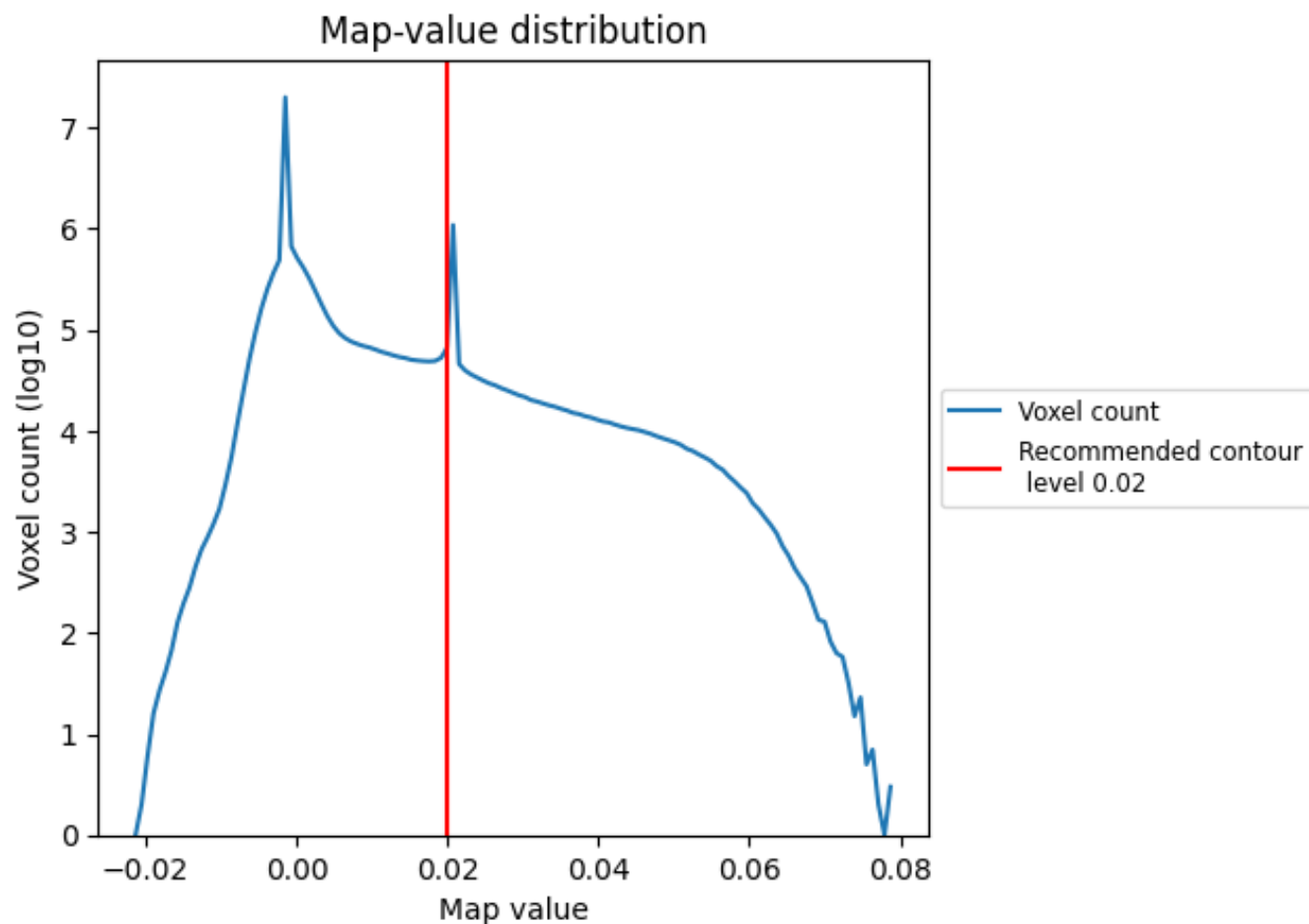
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

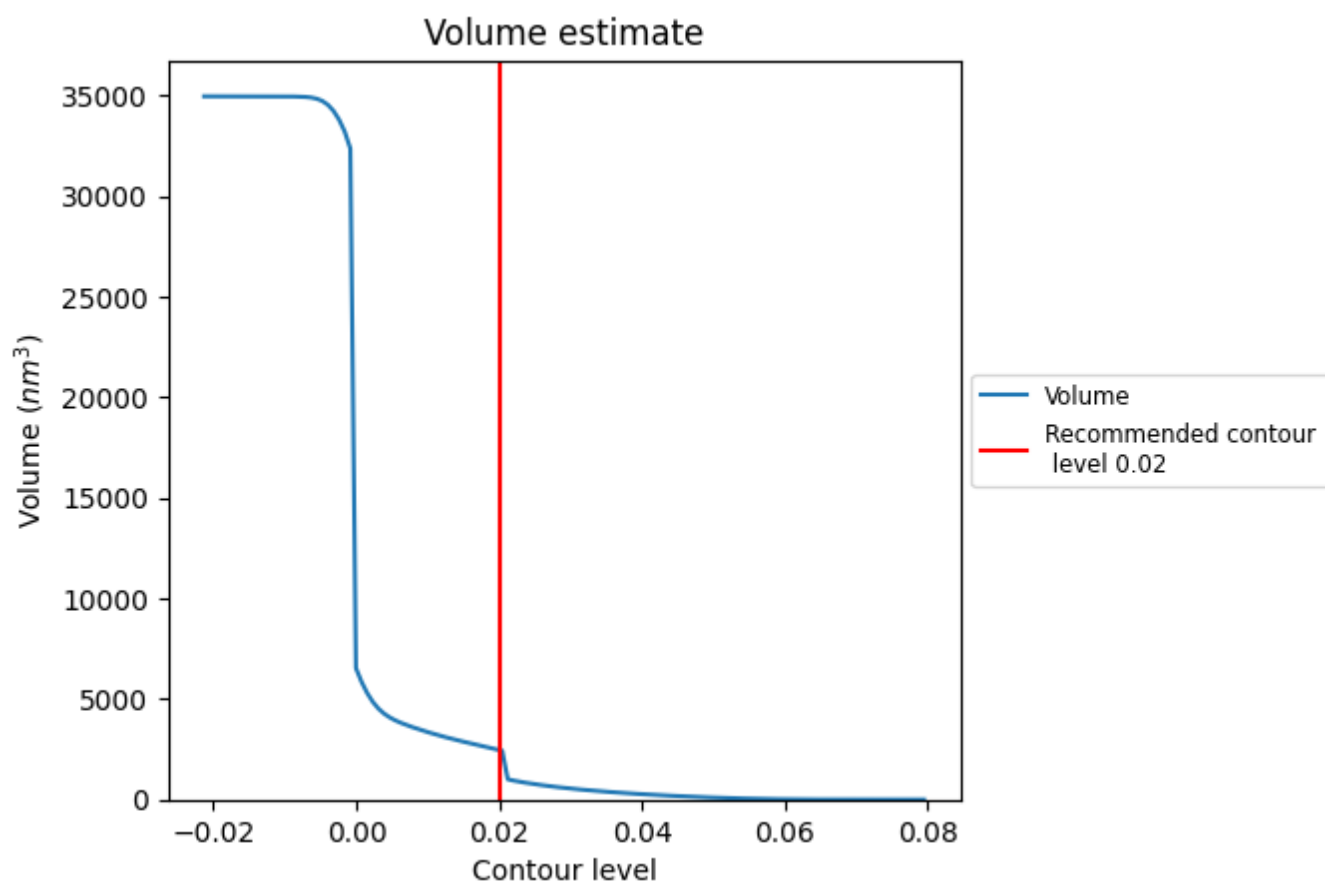
This section contains the results of statistical analysis of the map.

### 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.

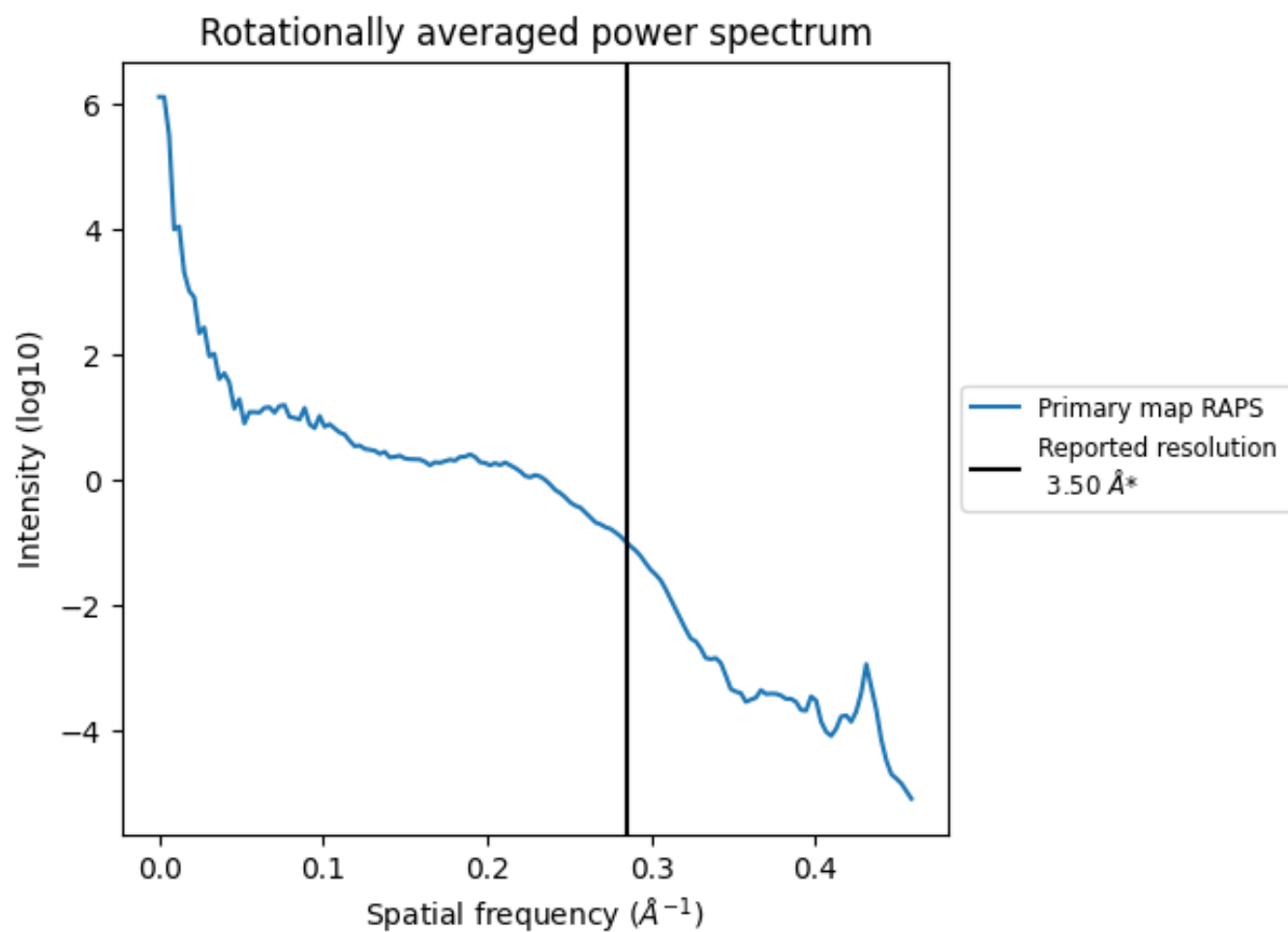
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2468 nm<sup>3</sup>; this corresponds to an approximate mass of 2229 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

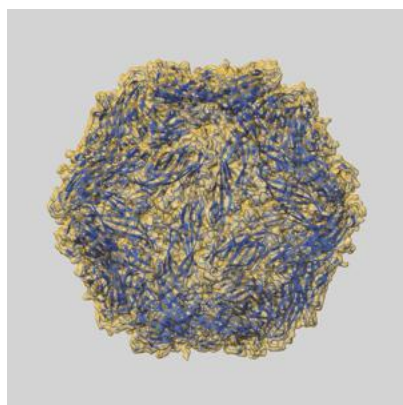
## 8 Fourier-Shell correlation ⓘ

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

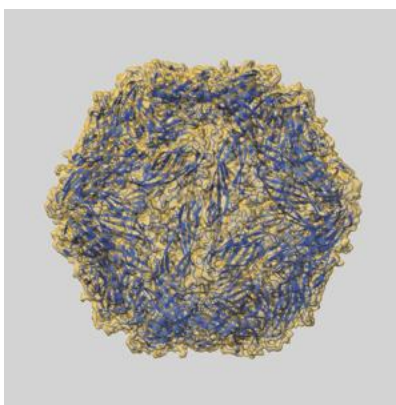
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8975 and PDB model 6E39. Per-residue inclusion information can be found in section 3 on page 10.

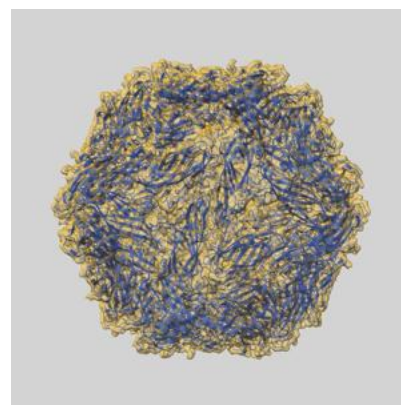
### 9.1 Map-model overlay [i](#)



X



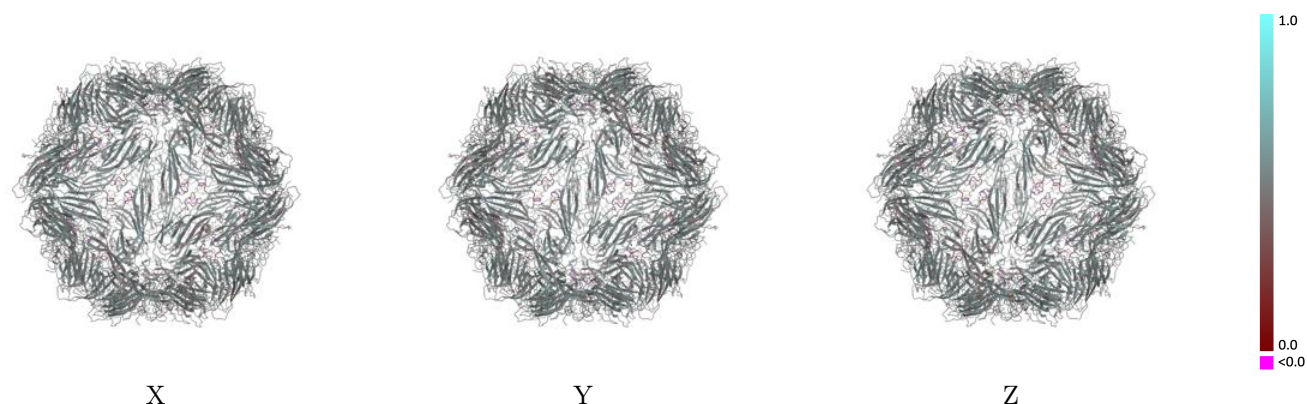
Y



Z

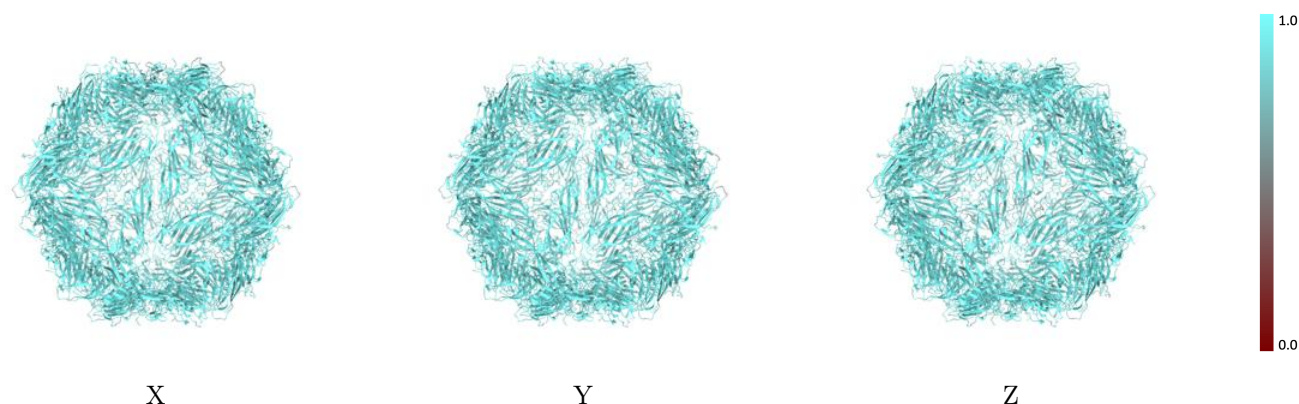
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



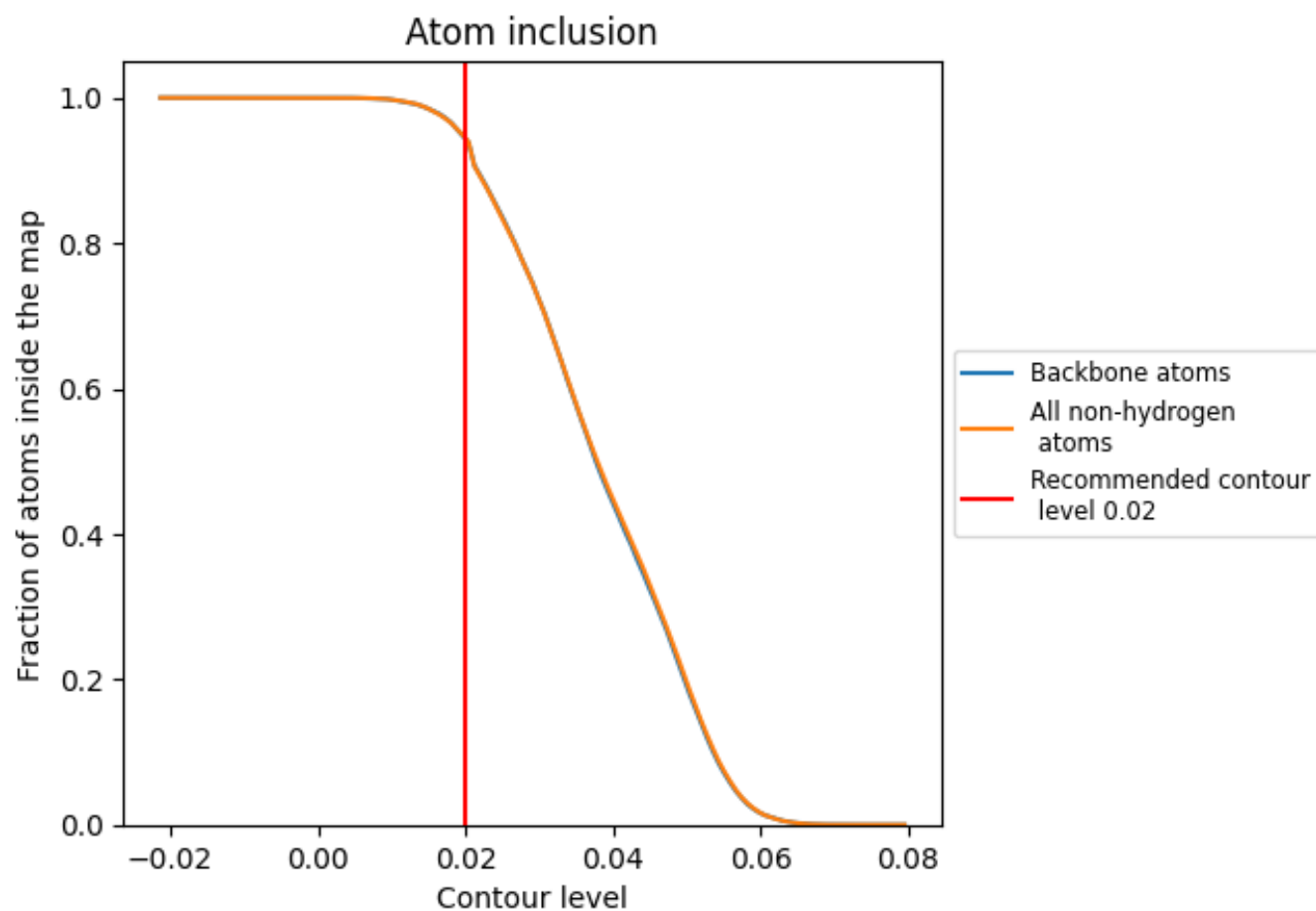
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.02) and Q-score for the entire model and for each chain.























































Chain	Atom inclusion	Q-score
All	 0.9447	 0.4840
A	 0.6389	 0.0080
A1	 0.9343	 0.4880
A2	 0.9396	 0.4660
A3	 0.9522	 0.4840
A4	 0.9549	 0.4890
A5	 0.9509	 0.4910
A6	 0.9237	 0.4720
A7	 0.9443	 0.4740
A8	 0.9529	 0.4850
A9	 0.9536	 0.4960
AA	 0.9323	 0.4900
AB	 0.9489	 0.4920
AC	 0.9469	 0.4720
AD	 0.9562	 0.4870
AE	 0.9456	 0.4810
AF	 0.9376	 0.4650
AG	 0.9522	 0.4950
AH	 0.9516	 0.4840
AI	 0.9516	 0.4740
AJ	 0.9443	 0.4800
AK	 0.9509	 0.4890
AL	 0.9529	 0.4910
AM	 0.9522	 0.4820
AN	 0.9536	 0.4860
AO	 0.9549	 0.4920
AP	 0.9549	 0.4910
AQ	 0.9575	 0.4940
AR	 0.9436	 0.4720
AS	 0.9489	 0.4840
AT	 0.9423	 0.4690
AU	 0.9409	 0.4630
AV	 0.9562	 0.4950
AW	 0.9409	 0.4780
AX	 0.9542	 0.4910



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Chain	Atom inclusion	Q-score
AY	 0.9496	 0.4770
AZ	 0.9569	 0.4920
Aa	 0.9542	 0.4940
Ab	 0.9496	 0.4800
Ac	 0.9555	 0.4890
Ad	 0.9443	 0.4670
Ae	 0.9443	 0.4680
Af	 0.9569	 0.4940
Ag	 0.9429	 0.4650
Ah	 0.9476	 0.4860
Ai	 0.9536	 0.4910
Aj	 0.9549	 0.4890
Ak	 0.9562	 0.4950
Al	 0.9529	 0.4920
Am	 0.9536	 0.4890
An	 0.9469	 0.4700
Ao	 0.9589	 0.4960
Ap	 0.9549	 0.4930
Aq	 0.9509	 0.4940
Ar	 0.9522	 0.4920
As	 0.9456	 0.4740
At	 0.9509	 0.4920
Au	 0.9569	 0.4940
Av	 0.9509	 0.4820
Aw	 0.9582	 0.4940
Ax	 0.9516	 0.4940
Ay	 0.9317	 0.4380