Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 12:04 PM EST

PDB ID	:	6E32
EMDB ID	:	EMD-8973
Title	:	Capsid protein of PCV2 with N,O6-DISULFO-GLUCOSAMINE
Authors	:	Khayat, R.; Dhindwal, S.
Deposited on	:	2018-07-13
Resolution	:	3.40 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:

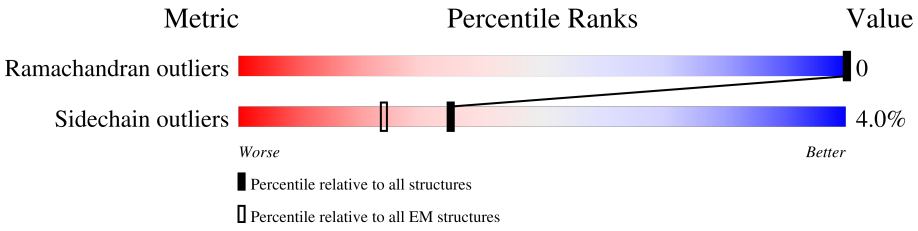
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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 >=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 <=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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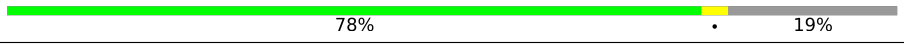
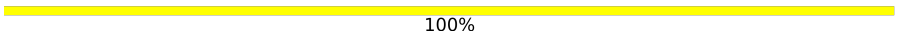
Mol	Chain	Length	Quality of chain
1	Ay	233	
2	A	5	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 183270 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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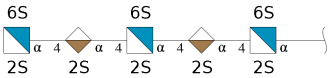
Mol	Chain	Residues	Atoms						AltConf	Trace
1	Ay	189	Total	C	H	N	O	S	0	0
			3053	995	1503	268	283	4		

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



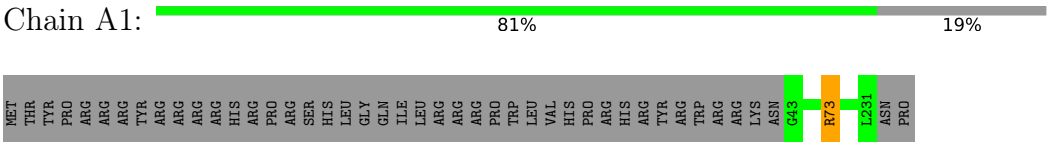
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	5	Total	C	N	O	S	0	0
			90	30	3	49	8		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

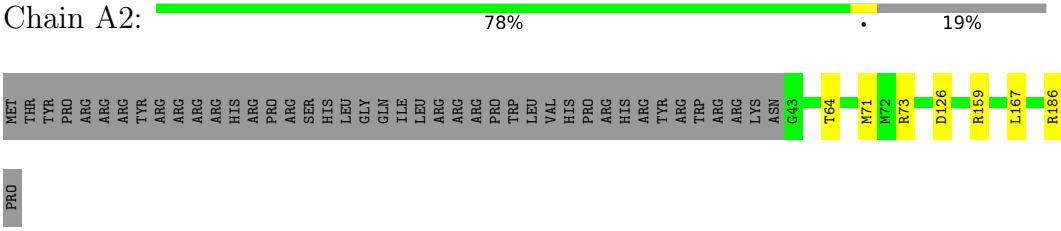
• Molecule 1: Capsid protein of PCV2

Chain A1:



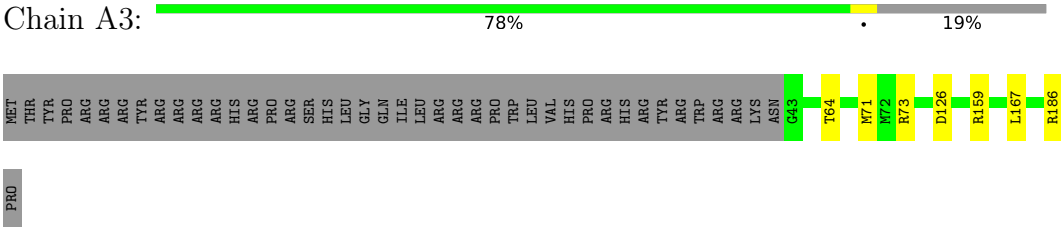
• Molecule 1: Capsid protein of PCV2

Chain A2:



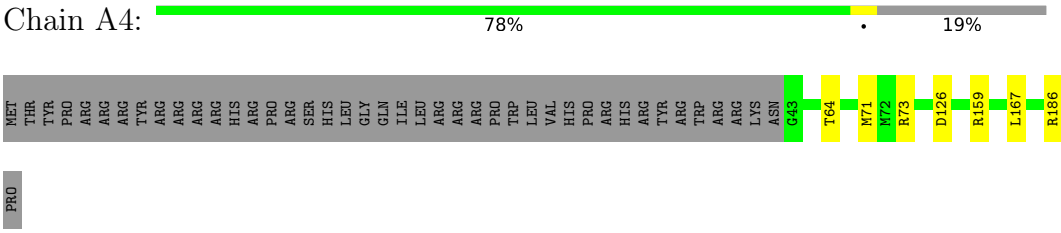
• Molecule 1: Capsid protein of PCV2

Chain A3:



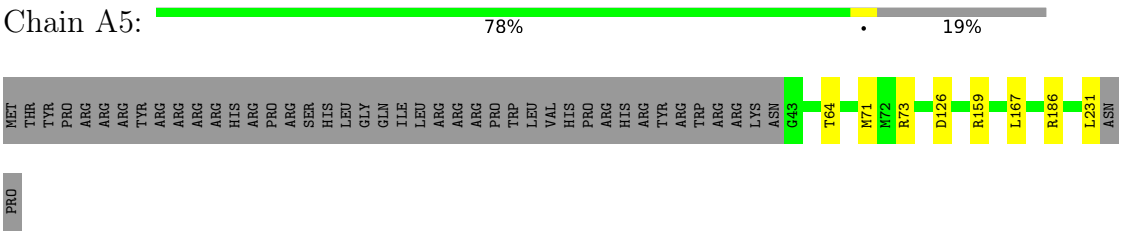
• Molecule 1: Capsid protein of PCV2

Chain A4:



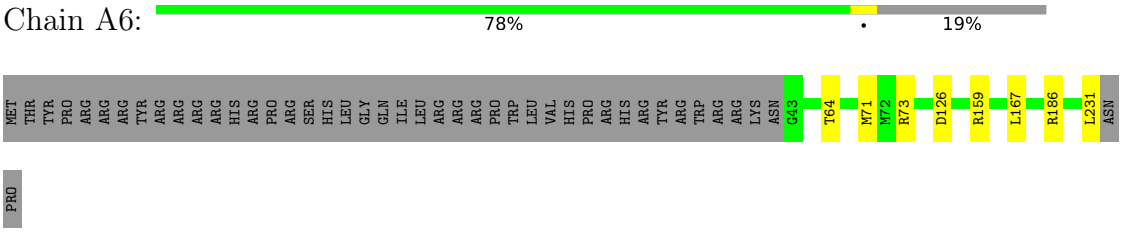
• Molecule 1: Capsid protein of PCV2

Chain A5:



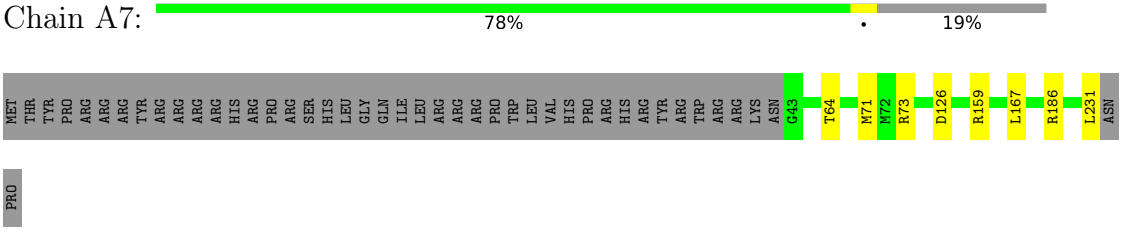
• Molecule 1: Capsid protein of PCV2

Chain A6:



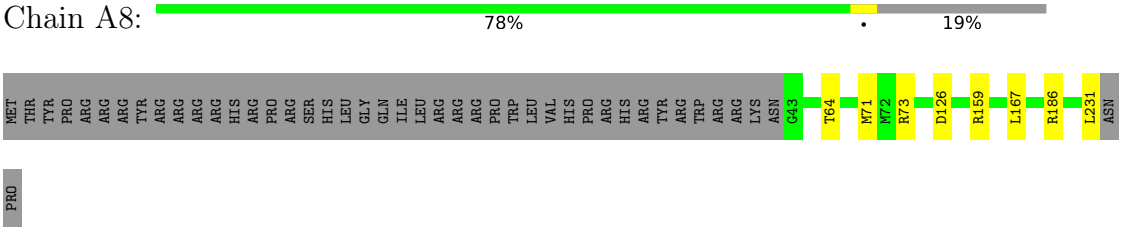
• Molecule 1: Capsid protein of PCV2

Chain A7:



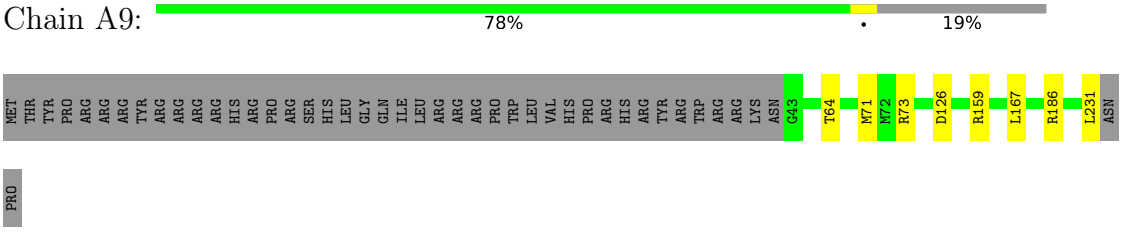
• Molecule 1: Capsid protein of PCV2

Chain A8:



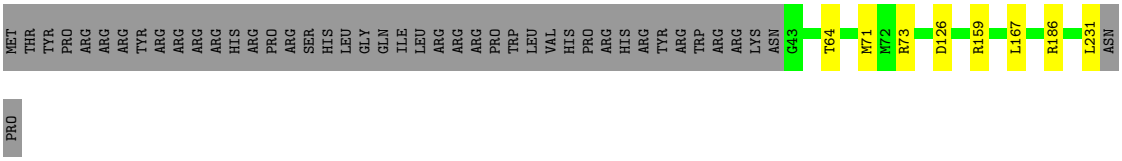
• Molecule 1: Capsid protein of PCV2

Chain A9:



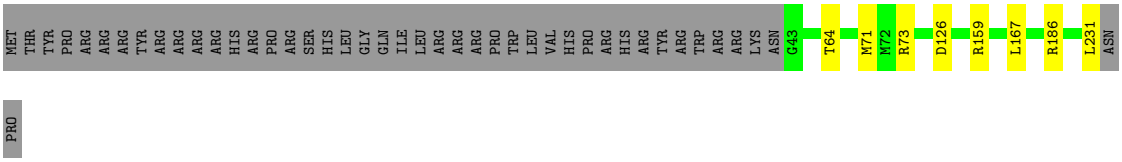
• Molecule 1: Capsid protein of PCV2

Chain AA:



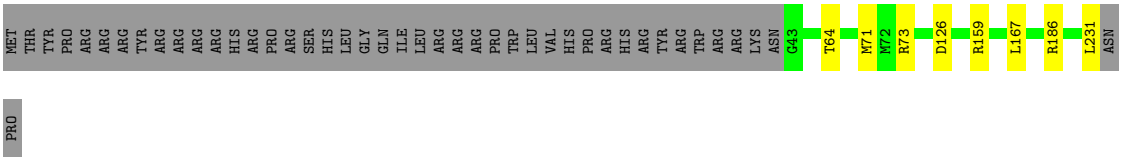
• Molecule 1: Capsid protein of PCV2

Chain AB:



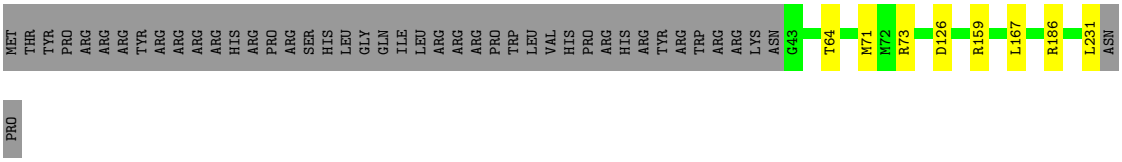
• Molecule 1: Capsid protein of PCV2

Chain AC:



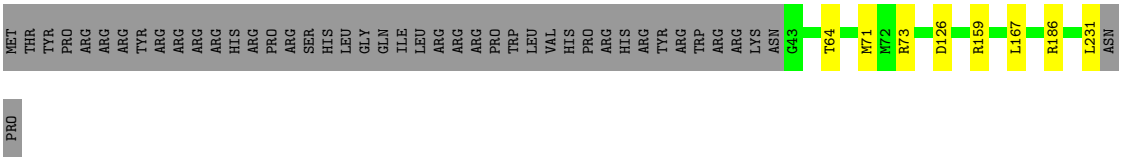
• Molecule 1: Capsid protein of PCV2

Chain AD:



• Molecule 1: Capsid protein of PCV2

Chain AE:

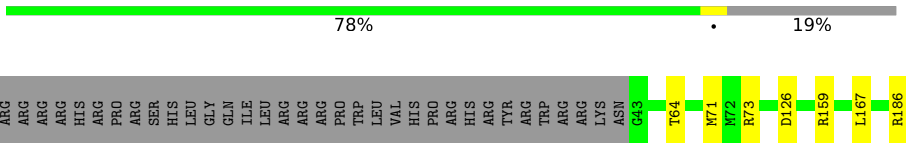


• Molecule 1: Capsid protein of PCV2

Chain AF:

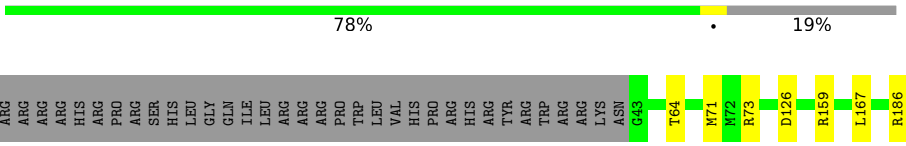
• Molecule 1: Capsid protein of PCV2

Chain AG:



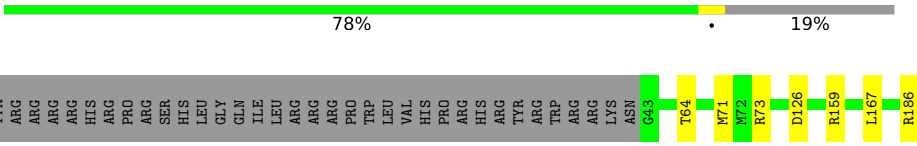
• Molecule 1: Capsid protein of PCV2

Chain AH:



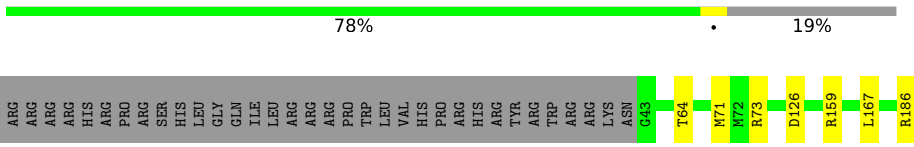
• Molecule 1: Capsid protein of PCV2

Chain AI:



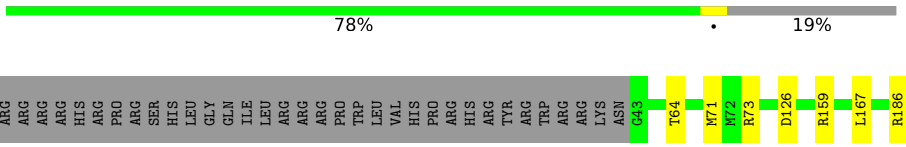
• Molecule 1: Capsid protein of PCV2

Chain AJ:



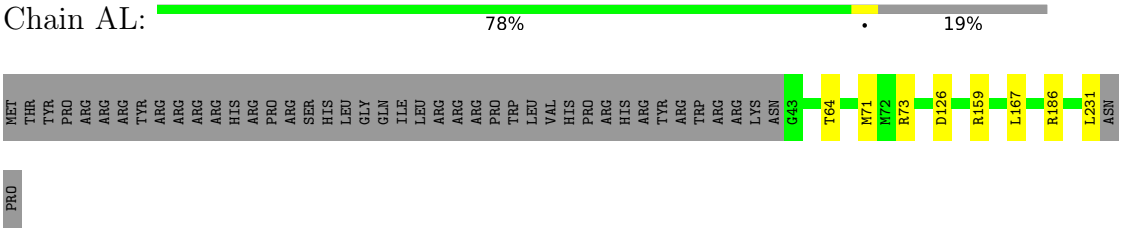
• Molecule 1: Capsid protein of PCV2

Chain AK:



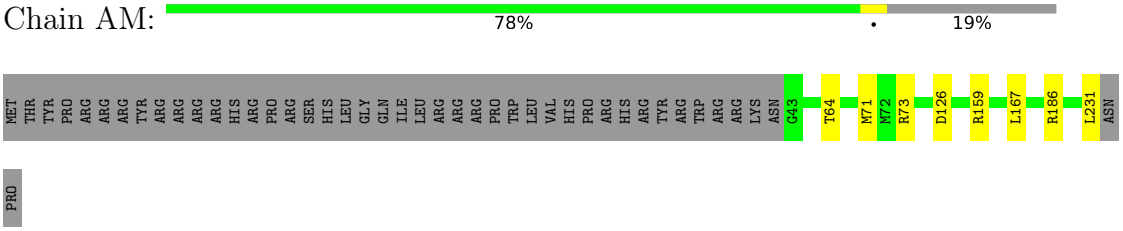
• Molecule 1: Capsid protein of PCV2

Chain AL:



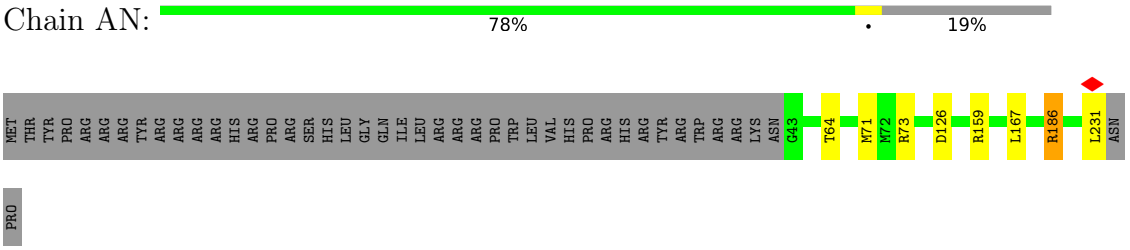
• Molecule 1: Capsid protein of PCV2

Chain AM:



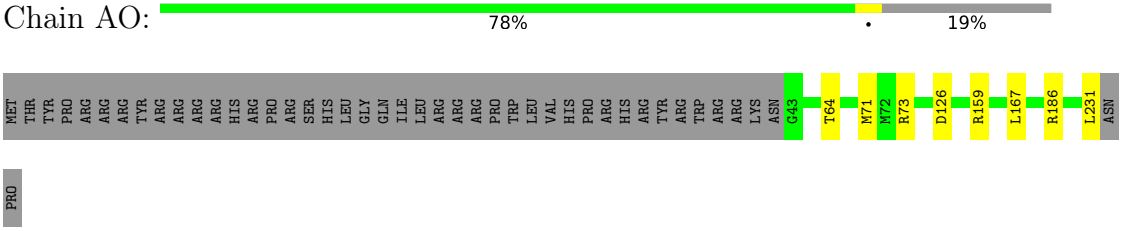
• Molecule 1: Capsid protein of PCV2

Chain AN:



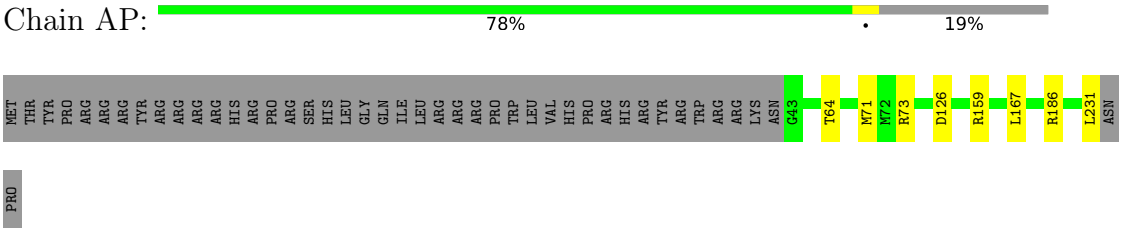
• Molecule 1: Capsid protein of PCV2

Chain AO:



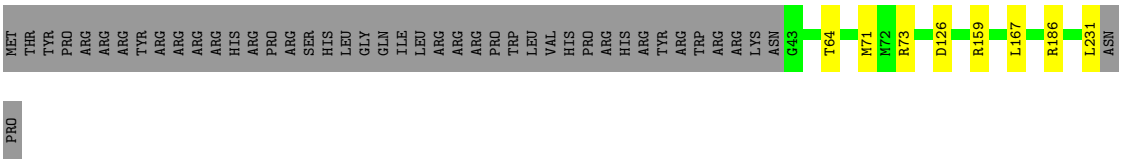
• Molecule 1: Capsid protein of PCV2

Chain AP:



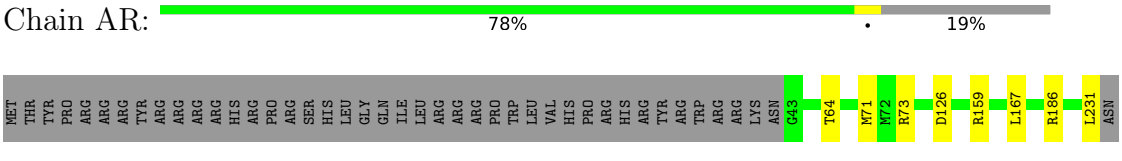
• Molecule 1: Capsid protein of PCV2

Chain AQ:



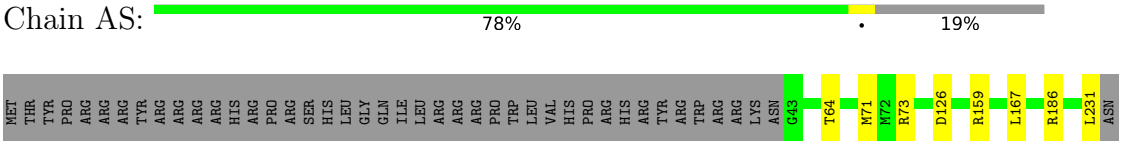
• Molecule 1: Capsid protein of PCV2

Chain AR:



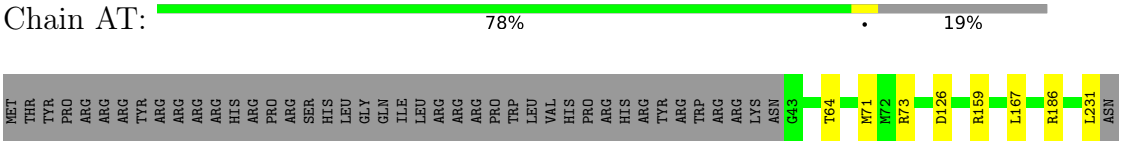
• Molecule 1: Capsid protein of PCV2

Chain AS:



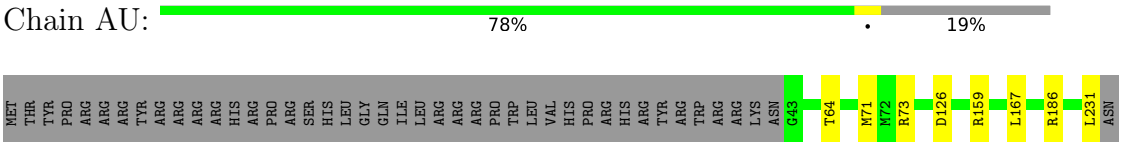
• Molecule 1: Capsid protein of PCV2

Chain AT:



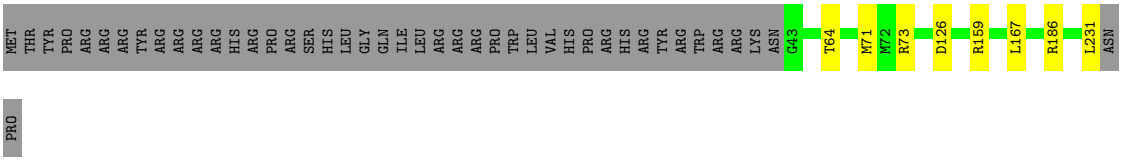
• Molecule 1: Capsid protein of PCV2

Chain AU:



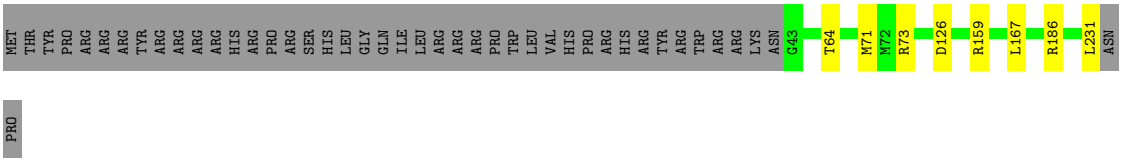
• Molecule 1: Capsid protein of PCV2

Chain AV:



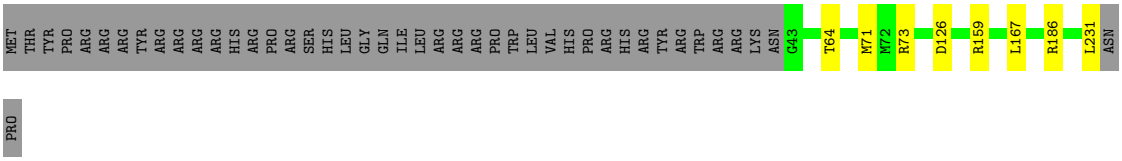
• Molecule 1: Capsid protein of PCV2

Chain AW:



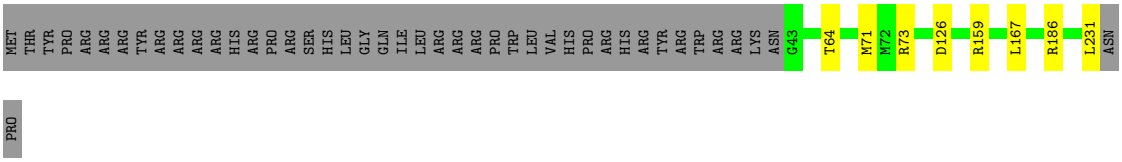
• Molecule 1: Capsid protein of PCV2

Chain AX:



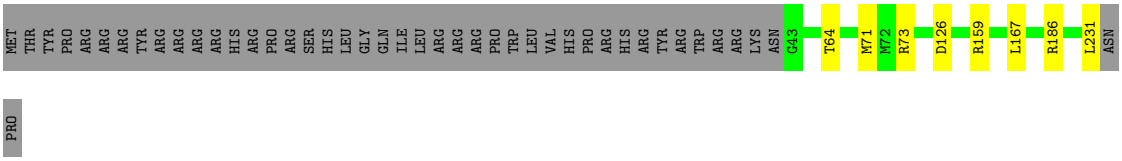
• Molecule 1: Capsid protein of PCV2

Chain AY:



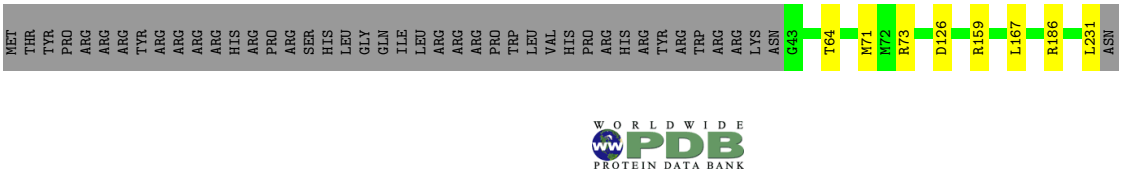
• Molecule 1: Capsid protein of PCV2

Chain AZ:



• Molecule 1: Capsid protein of PCV2

Chain Aa:



• Molecule 1: Capsid protein of PCV2

Chain Ab:

• Molecule 1: Capsid protein of PCV2

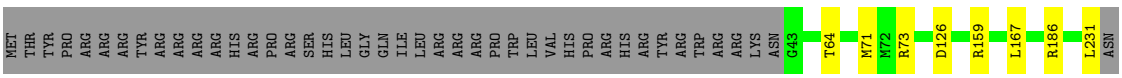
Chain Ac:

• Molecule 1: Capsid protein of PCV2

Chain Ad:

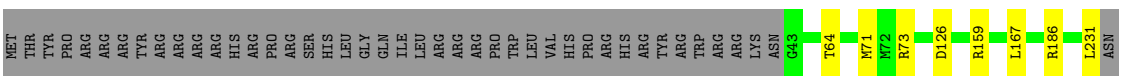
• Molecule 1: Capsid protein of PCV2

Chain Ae:



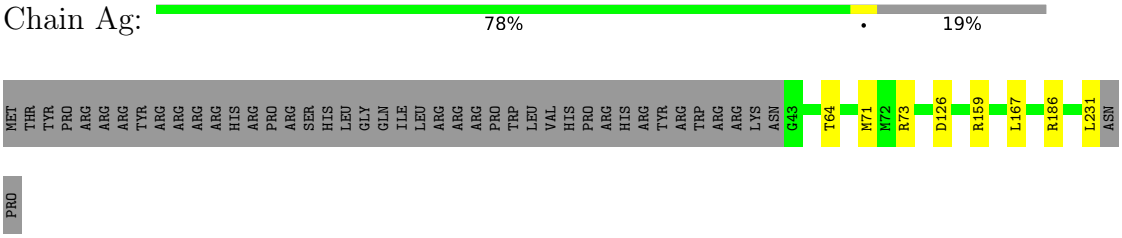
• Molecule 1: Capsid protein of PCV2

Chain Af:



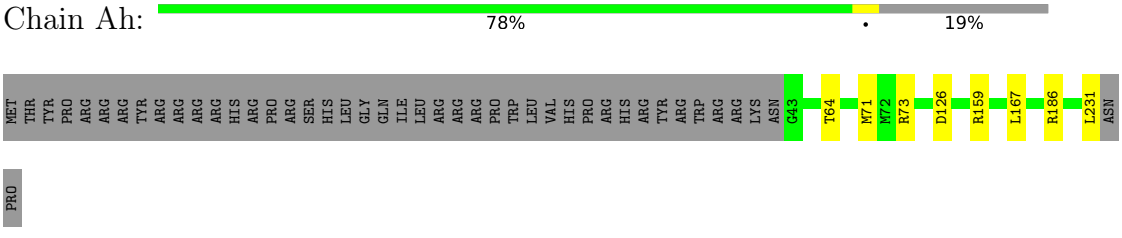
• Molecule 1: Capsid protein of PCV2

Chain Ag:



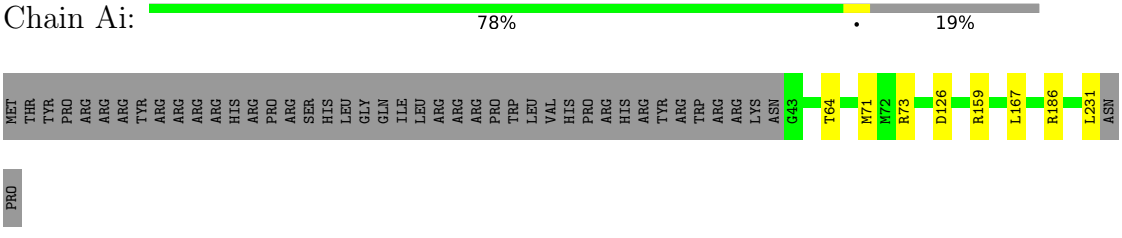
• Molecule 1: Capsid protein of PCV2

Chain Ah:



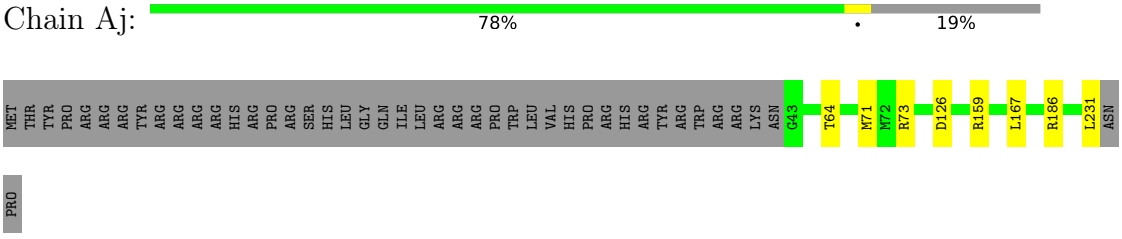
• Molecule 1: Capsid protein of PCV2

Chain Ai:



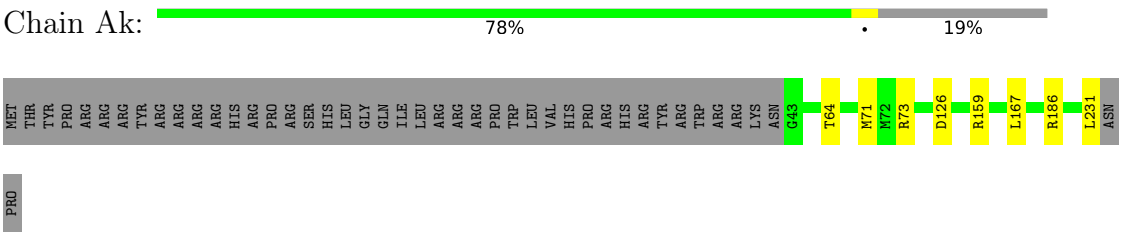
• Molecule 1: Capsid protein of PCV2

Chain Aj:



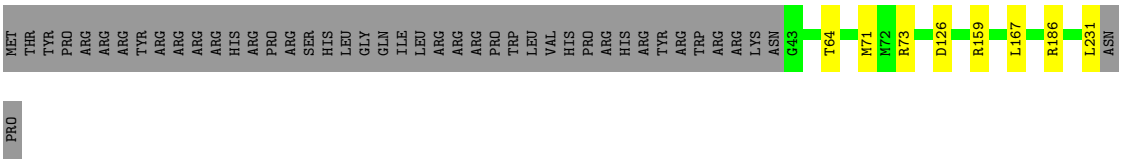
• Molecule 1: Capsid protein of PCV2

Chain Ak:



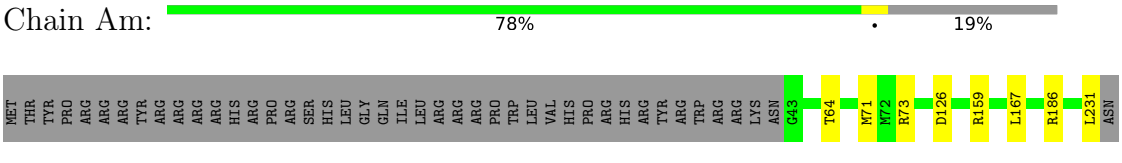
• Molecule 1: Capsid protein of PCV2

Chain Al:



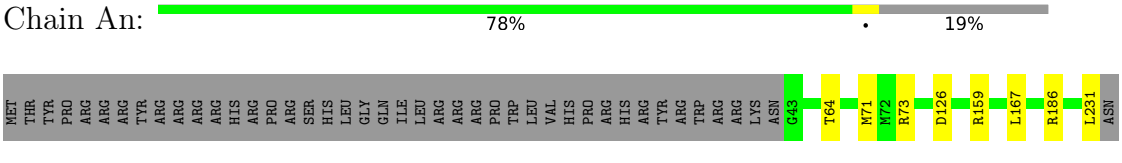
• Molecule 1: Capsid protein of PCV2

Chain Am:



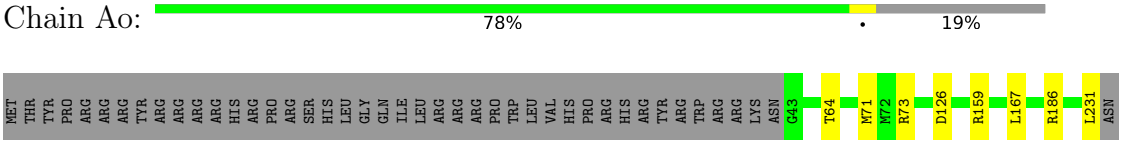
• Molecule 1: Capsid protein of PCV2

Chain An:



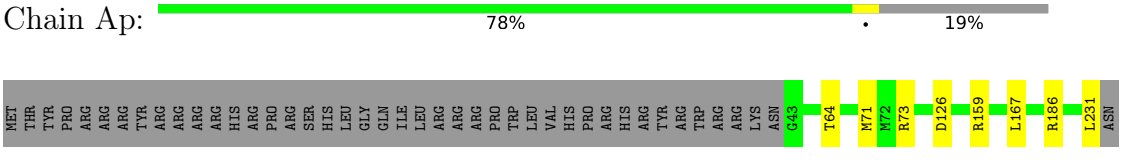
• Molecule 1: Capsid protein of PCV2

Chain Ao:



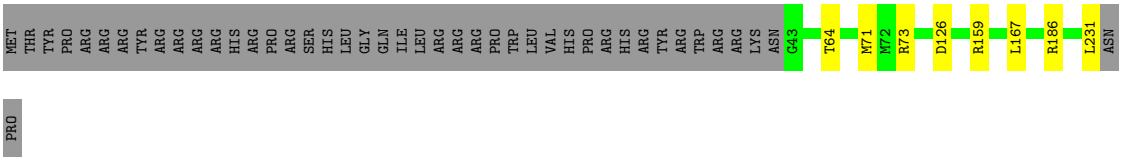
• Molecule 1: Capsid protein of PCV2

Chain Ap:



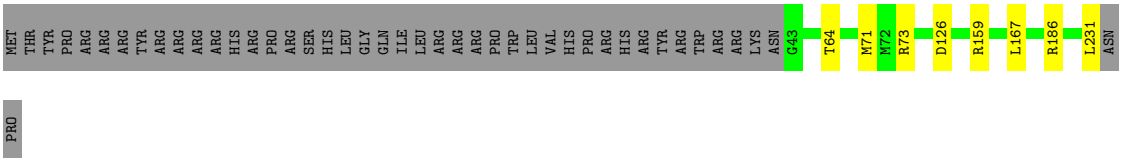
• Molecule 1: Capsid protein of PCV2

Chain Aq:



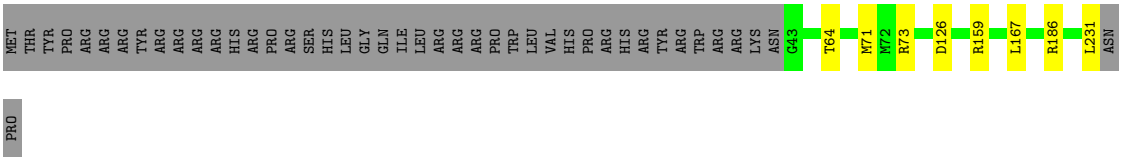
• Molecule 1: Capsid protein of PCV2

Chain Ar:



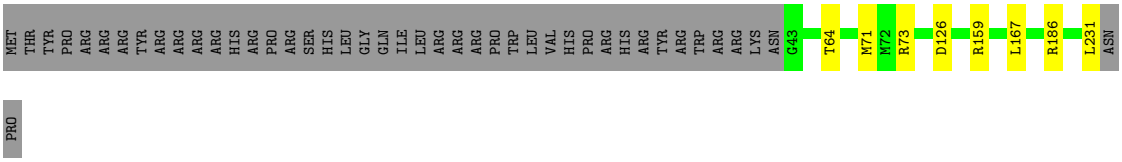
• Molecule 1: Capsid protein of PCV2

Chain As:



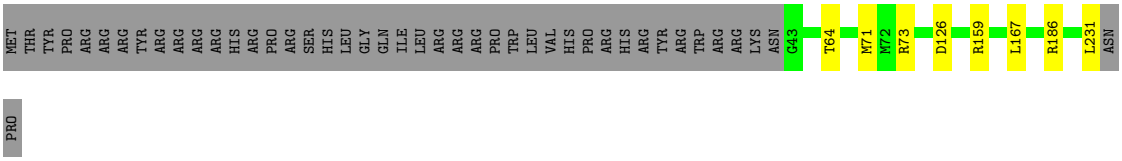
• Molecule 1: Capsid protein of PCV2

Chain At:



• Molecule 1: Capsid protein of PCV2

Chain Au:



• Molecule 1: Capsid protein of PCV2

Chain Av:

• Molecule 1: Capsid protein of PCV2

Chain Aw:

• Molecule 1: Capsid protein of PCV2

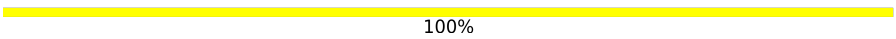
Chain Ax:

• Molecule 1: Capsid protein of PCV2

Chain Ay:

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

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	114389	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 ($e^-/Å^2$)	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	-0.022	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	0.44	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	A1	0	1
1	AN	0	1
All	All	0	2

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A1	73	ARG	Sidechain
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%)	176 (94%)	11 (6%)	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%)	10837 (97%)	383 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	172/215 (80%)	171 (99%)	1 (1%)	86	94
1	A2	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A3	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A4	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A5	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A6	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A7	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A8	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	A9	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AA	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AB	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AC	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AD	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AE	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AF	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AG	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AH	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AI	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AJ	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AK	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AL	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AM	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AN	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AO	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AP	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AQ	172/215 (80%)	165 (96%)	7 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AR	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AS	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AT	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AU	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AV	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AW	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AX	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AY	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	AZ	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Aa	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ab	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ac	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ad	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ae	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Af	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ag	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ah	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ai	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Aj	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ak	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Al	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Am	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	An	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ao	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ap	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Aq	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Ar	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	As	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	At	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Au	172/215 (80%)	165 (96%)	7 (4%)	30	59
1	Av	172/215 (80%)	165 (96%)	7 (4%)	30	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Aw	172/215 (80%)	165 (96%)	7 (4%)	30 59
1	Ax	172/215 (80%)	165 (96%)	7 (4%)	30 59
1	Ay	172/215 (80%)	165 (96%)	7 (4%)	30 59
All	All	10320/12900 (80%)	9906 (96%)	414 (4%)	35 60

All (414) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	73	ARG
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

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Mol	Chain	Res	Type
1	A6	167	LEU
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	Ay	167	LEU
1	Ay	186	ARG
1	Ay	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
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
1	AP	212	ASN

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Mol	Chain	Res	Type
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
1	Ay	212	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)

5 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	SGN	A	1	2	19,20,20	3.61	5 (26%)	24,31,31	1.89	7 (29%)
2	IDS	A	2	2	16,16,17	1.25	1 (6%)	17,24,26	0.96	0
2	SGN	A	3	2	18,19,20	3.75	5 (27%)	22,29,31	1.71	5 (22%)
2	IDS	A	4	2	16,16,17	1.27	1 (6%)	17,24,26	1.03	0
2	SGN	A	5	2	18,19,20	3.76	5 (27%)	22,29,31	1.50	3 (13%)

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	SGN	A	1	2	-	3/11/31/31	0/1/1/1
2	IDS	A	2	2	-	0/9/26/29	0/1/1/1
2	SGN	A	3	2	-	3/11/28/31	0/1/1/1
2	IDS	A	4	2	-	5/9/26/29	0/1/1/1
2	SGN	A	5	2	-	5/11/28/31	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	SGN	S1-N2	14.63	1.79	1.59
2	A	5	SGN	S1-N2	14.54	1.79	1.59
2	A	1	SGN	S1-N2	14.52	1.79	1.59
2	A	5	SGN	O1S-S1	3.06	1.45	1.42
2	A	5	SGN	O2S-S1	3.05	1.45	1.42
2	A	1	SGN	O2S-S1	2.96	1.45	1.42
2	A	3	SGN	O2S-S1	2.86	1.45	1.42
2	A	3	SGN	O1S-S1	2.77	1.45	1.42
2	A	1	SGN	O1S-S1	2.75	1.45	1.42
2	A	2	IDS	C1-C2	2.71	1.56	1.51
2	A	4	IDS	C1-C2	2.63	1.55	1.51
2	A	5	SGN	C1-C2	2.58	1.56	1.52
2	A	3	SGN	C1-C2	2.29	1.55	1.52
2	A	1	SGN	C1-C2	2.23	1.55	1.52
2	A	1	SGN	O6-S2	-2.22	1.50	1.56
2	A	3	SGN	O6-S2	-2.09	1.51	1.56
2	A	5	SGN	O6-S2	-2.02	1.51	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	SGN	O1S-S1-O2S	-3.99	110.74	120.16
2	A	3	SGN	O2S-S1-N2	-3.45	102.58	108.87
2	A	1	SGN	O1-C1-C2	3.42	116.32	109.22
2	A	1	SGN	O2S-S1-N2	-3.12	103.17	108.87
2	A	5	SGN	O2S-S1-N2	-3.12	103.17	108.87
2	A	1	SGN	O1S-S1-N2	-3.06	103.28	108.87
2	A	3	SGN	O1S-S1-O2S	-2.96	113.17	120.16
2	A	3	SGN	O6-C6-C5	2.75	112.74	107.62
2	A	3	SGN	C3-C4-C5	-2.50	105.78	110.24
2	A	1	SGN	O5-C1-C2	2.45	111.98	109.52
2	A	1	SGN	C3-C4-C5	-2.43	105.91	110.24
2	A	3	SGN	O4-C4-C5	2.38	115.22	109.30
2	A	5	SGN	C4-C3-C2	-2.37	107.55	111.02
2	A	1	SGN	O4-C4-C3	2.20	115.43	110.35
2	A	5	SGN	O4-C4-C3	2.16	115.34	110.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	SGN	C2-N2-S1-O1S

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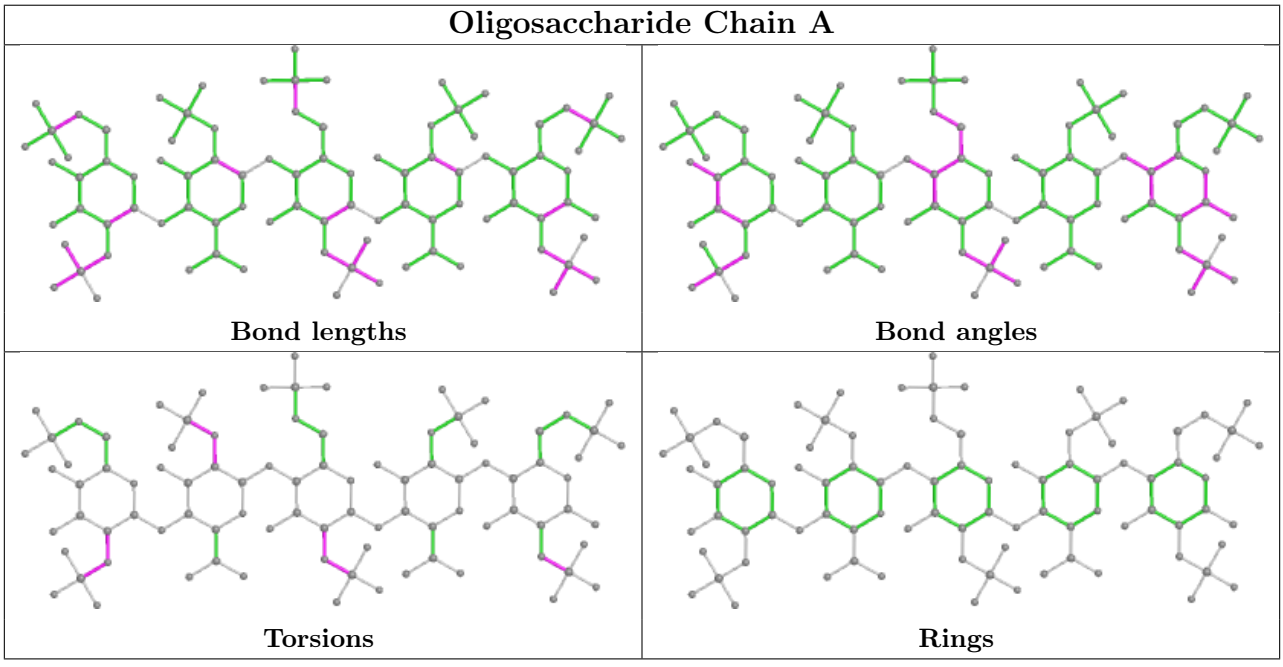
Mol	Chain	Res	Type	Atoms
2	A	1	SGN	C2-N2-S1-O2S
2	A	1	SGN	C2-N2-S1-O3S
2	A	3	SGN	C2-N2-S1-O2S
2	A	4	IDS	C1-C2-O2-S
2	A	4	IDS	C3-C2-O2-S
2	A	4	IDS	C2-O2-S-O3S
2	A	5	SGN	C2-N2-S1-O2S
2	A	5	SGN	C2-N2-S1-O3S
2	A	4	IDS	C2-O2-S-O1S
2	A	4	IDS	C2-O2-S-O2S
2	A	5	SGN	C2-N2-S1-O1S
2	A	5	SGN	C3-C2-N2-S1
2	A	3	SGN	C3-C2-N2-S1
2	A	3	SGN	C1-C2-N2-S1
2	A	5	SGN	C1-C2-N2-S1

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.

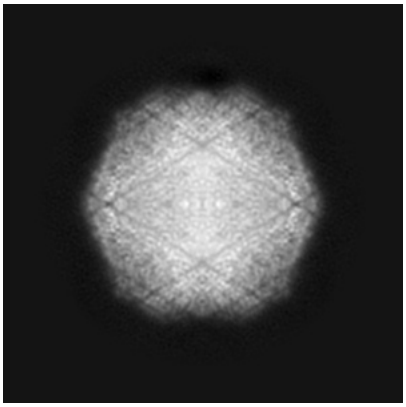
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8973. These allow visual inspection of the internal detail of the map and identification of artifacts.

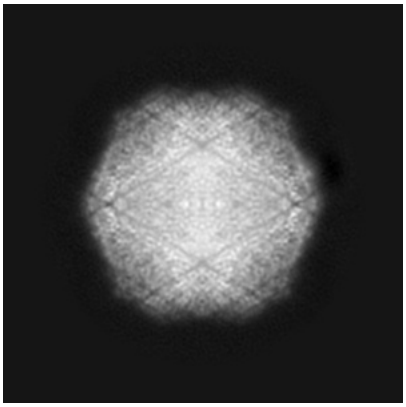
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

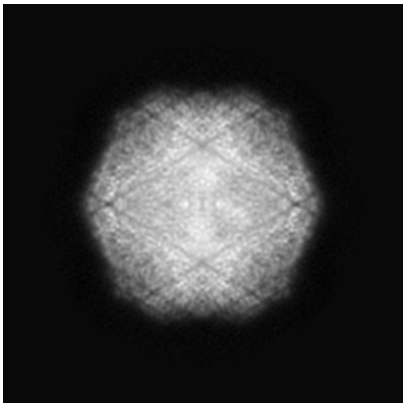
6.1.1 Primary map



X



Y

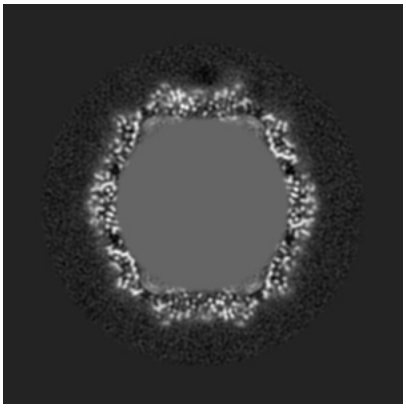


Z

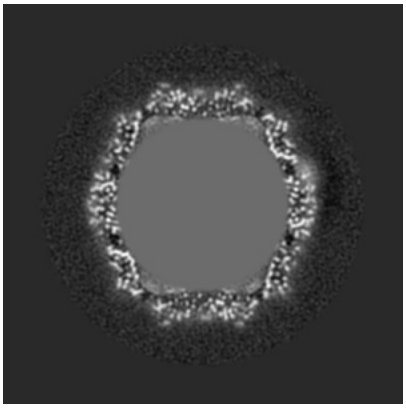
The images above show the map projected in three orthogonal directions.

6.2 Central slices

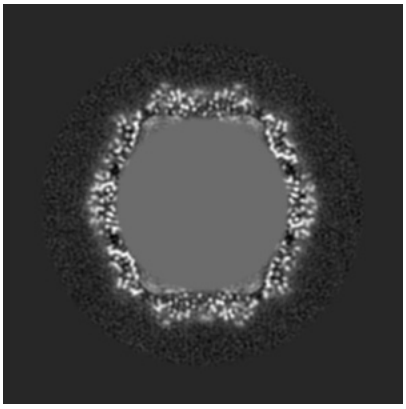
6.2.1 Primary map



X Index: 150



Y Index: 150

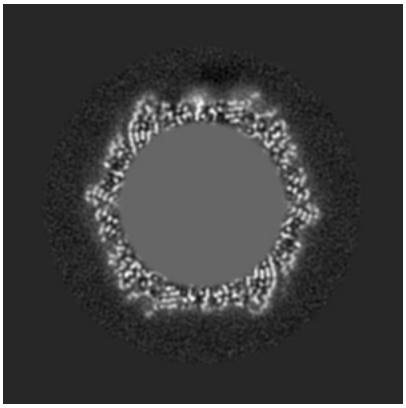


Z Index: 150

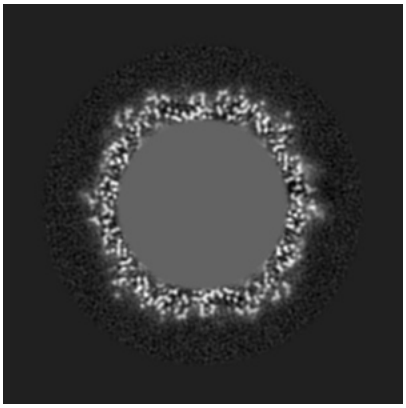
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

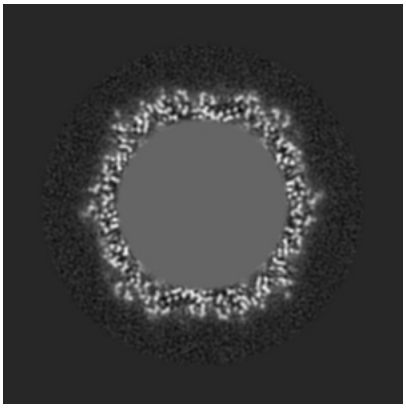
6.3.1 Primary map



X Index: 169



Y Index: 137

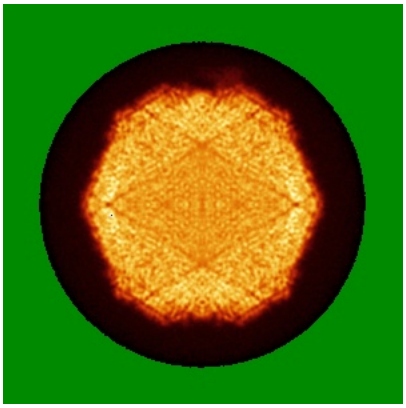


Z Index: 161

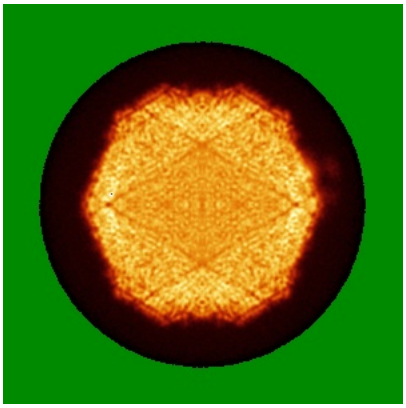
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

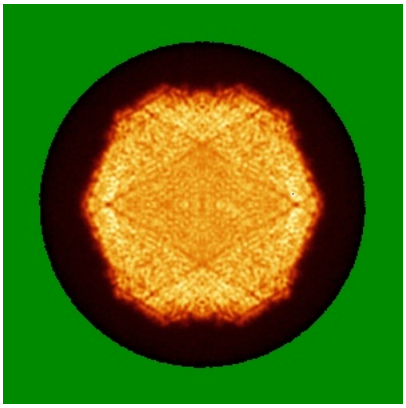
6.4.1 Primary map



X



Y

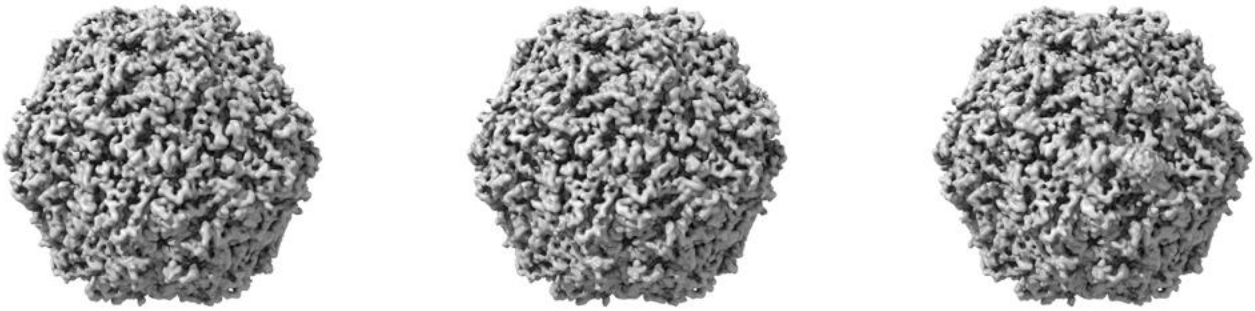


Z

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



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.

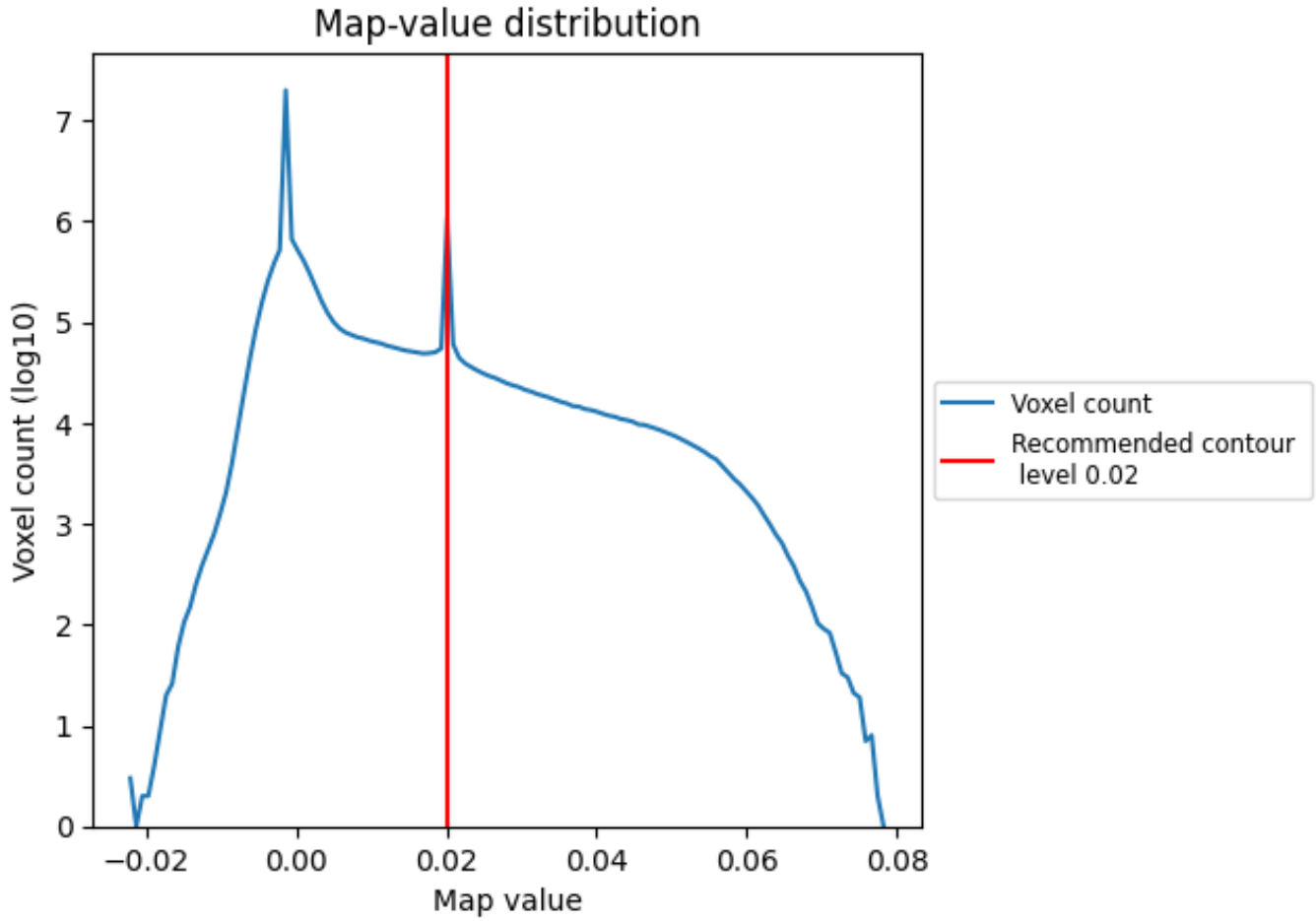
6.6 Mask visualisation (i)

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

7 Map analysis

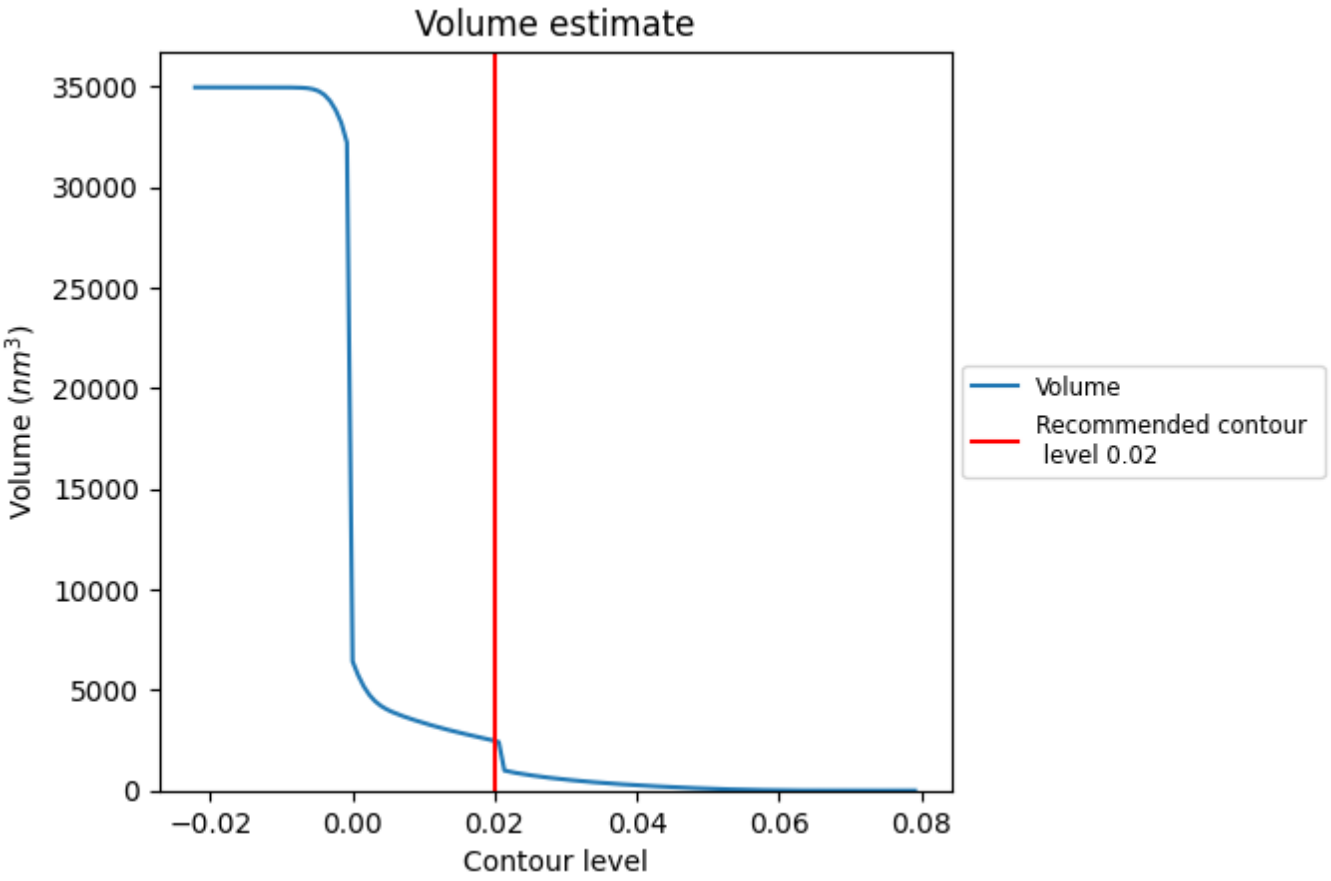
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

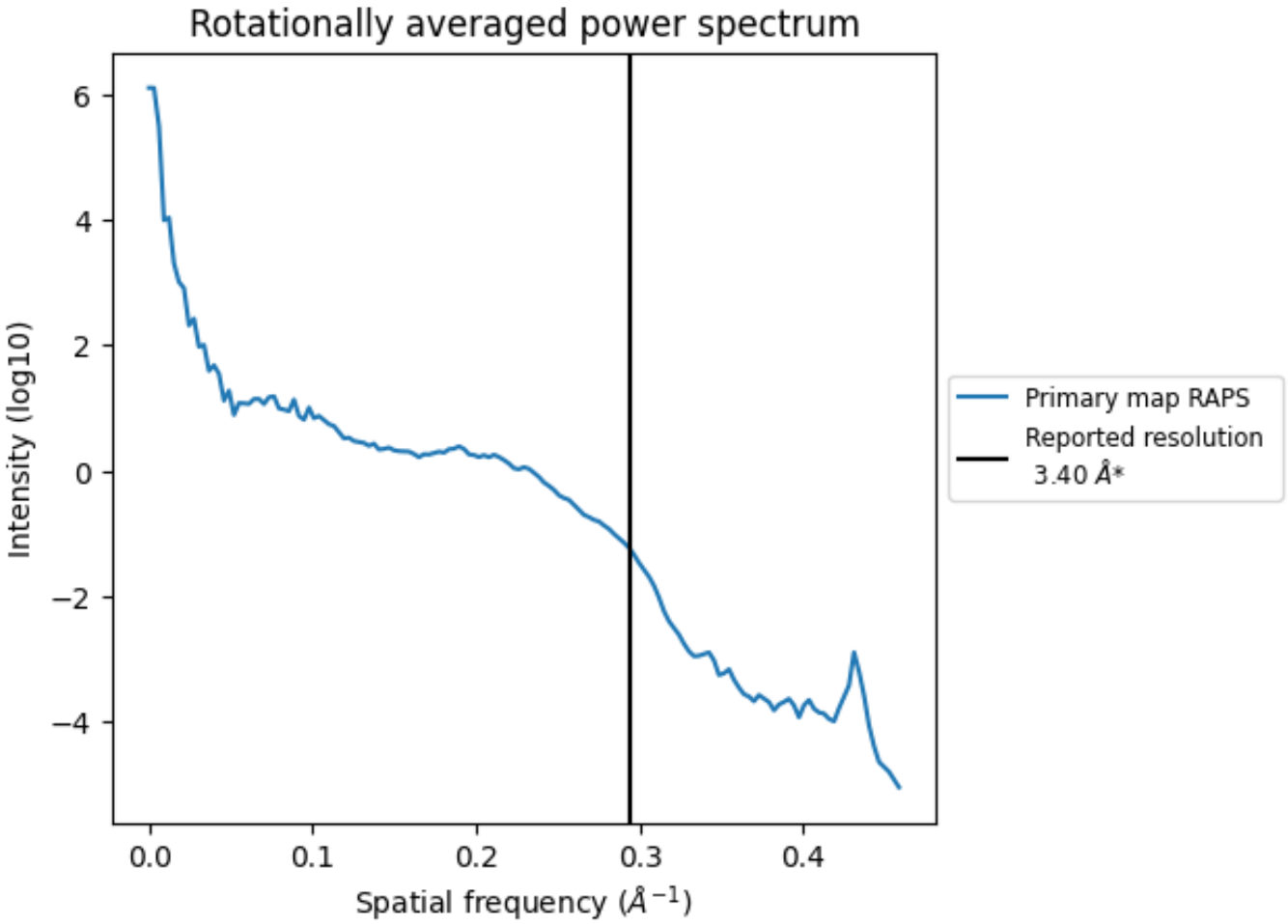
7.2 Volume estimate



The volume at the recommended contour level is 2468 nm^3; this corresponds to an approximate mass of 2230 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 0.294 Å^{-1}

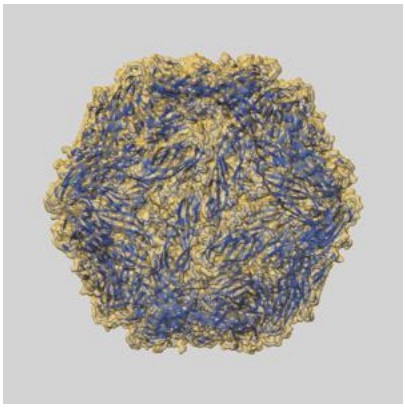
8 Fourier-Shell correlation (i)

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

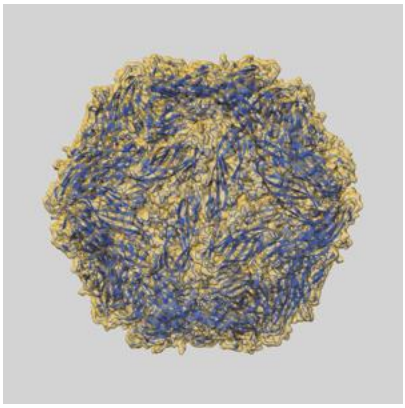
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8973 and PDB model 6E32. Per-residue inclusion information can be found in section 3 on page 10.

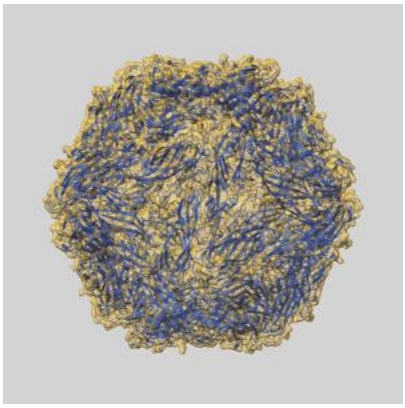
9.1 Map-model overlay



X



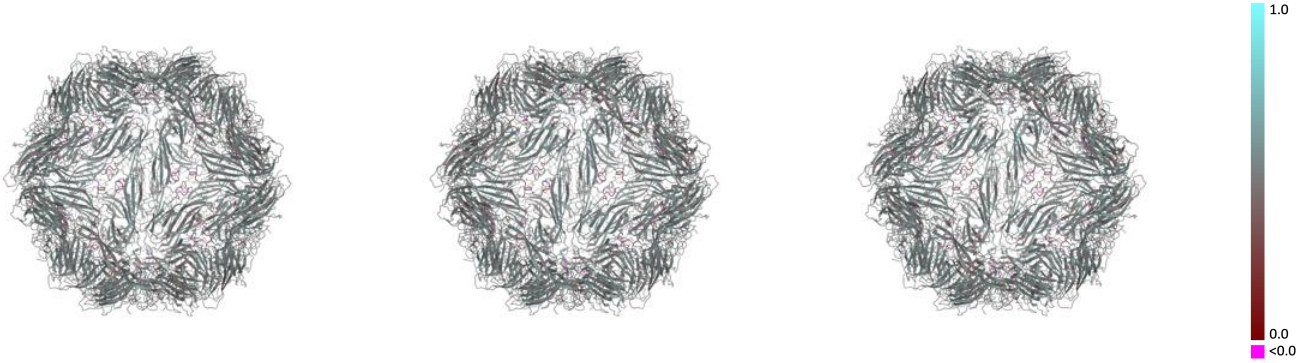
Y



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.

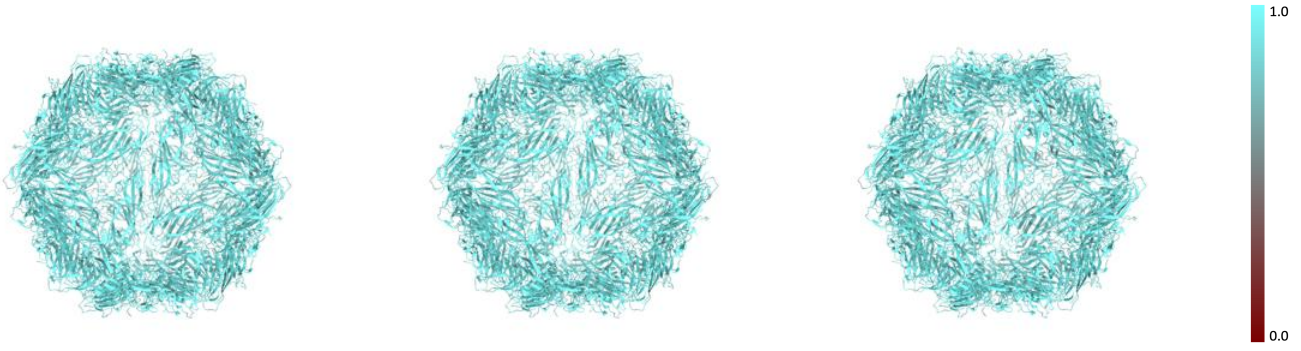
9.2 Q-score mapped to coordinate model



X Y Z

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

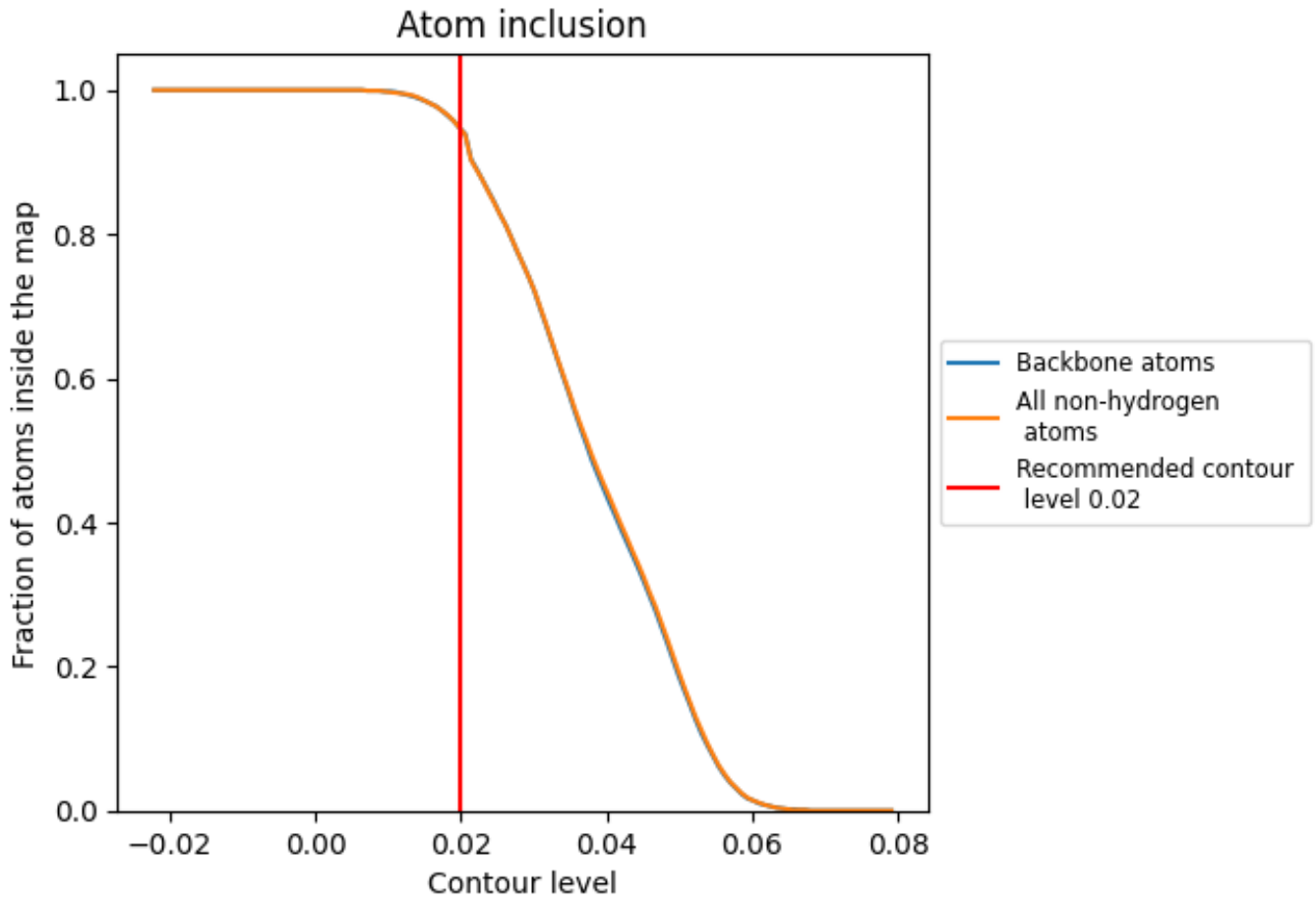
9.3 Atom inclusion mapped to coordinate model



X Y Z

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	0.9450	0.4840
A	0.6000	0.0640
A1	0.9480	0.4910
A2	0.9390	0.4670
A3	0.9510	0.4860
A4	0.9580	0.4890
A5	0.9420	0.4920
A6	0.9500	0.4730
A7	0.9460	0.4760
A8	0.9500	0.4860
A9	0.9560	0.4910
AA	0.9320	0.4860
AB	0.9500	0.4920
AC	0.9430	0.4710
AD	0.9550	0.4880
AE	0.9480	0.4840
AF	0.9400	0.4630
AG	0.9500	0.4960
AH	0.9500	0.4830
AI	0.9520	0.4780
AJ	0.9490	0.4800
AK	0.9510	0.4920
AL	0.9540	0.4910
AM	0.9480	0.4820
AN	0.9450	0.4880
AO	0.9500	0.4930
AP	0.9520	0.4900
AQ	0.9540	0.4930
AR	0.9470	0.4730
AS	0.9530	0.4850
AT	0.9440	0.4700
AU	0.9380	0.4660
AV	0.9530	0.4980
AW	0.9480	0.4770
AX	0.9540	0.4930

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Chain	Atom inclusion	Q-score
AY	0.9480	0.4780
AZ	0.9500	0.4910
Aa	0.9570	0.4940
Ab	0.9480	0.4810
Ac	0.9570	0.4900
Ad	0.9480	0.4730
Ae	0.9450	0.4700
Af	0.9540	0.4970
Ag	0.9440	0.4690
Ah	0.9580	0.4880
Ai	0.9560	0.4910
Aj	0.9500	0.4890
Ak	0.9590	0.4960
Al	0.9550	0.4910
Am	0.9500	0.4890
An	0.9430	0.4740
Ao	0.9490	0.4930
Ap	0.9560	0.4930
Aq	0.9510	0.4920
Ar	0.9600	0.4930
As	0.9460	0.4740
At	0.9560	0.4920
Au	0.9550	0.4950
Av	0.9530	0.4840
Aw	0.9550	0.4970
Ax	0.9540	0.4940
Ay	0.9350	0.4420