Full wwPDB EM Validation Report ⓘ

Mar 12, 2024 – 12:16 pm GMT

PDB ID	:	7QCN
EMDB ID	:	EMD-13897
Title	:	Structure of the MUCIN-2 Cterminal domains: vWCN to TIL domains with a C2 symmetry
Authors	:	Gallego, P.; Hansson, G.C.
Deposited on	:	2021-11-24
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:

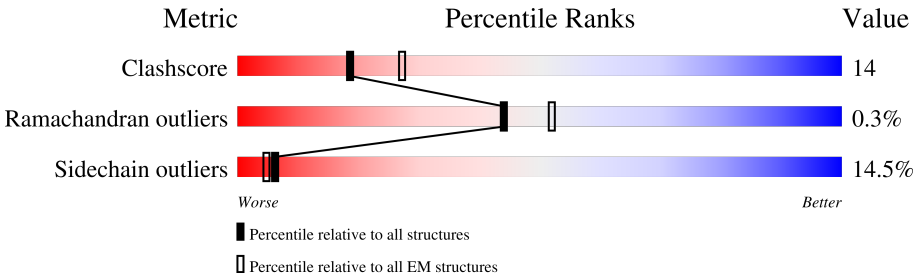
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	A	407	66% 29% 5%
1	B	407	65% 30% .
2	C	5	20% 80%
2	D	5	20% 80%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6416 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Mucin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	407	Total	C	N	O	S	0	0
			3104	1948	510	601	45		
1	B	407	Total	C	N	O	S	0	0
			3104	1948	510	601	45		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP Q02817
A	?	-	ASP	deletion	UNP Q02817
A	?	-	PRO	deletion	UNP Q02817
A	?	-	PRO	deletion	UNP Q02817
A	?	-	ARG	deletion	UNP Q02817
A	?	-	GLN	deletion	UNP Q02817
A	?	-	GLU	deletion	UNP Q02817
A	?	-	ASN	deletion	UNP Q02817
A	?	-	GLU	deletion	UNP Q02817
A	?	-	VAL	deletion	UNP Q02817
A	?	-	ASN	deletion	UNP Q02817
A	?	-	ARG	deletion	UNP Q02817
A	?	-	GLN	deletion	UNP Q02817
A	?	-	HIS	deletion	UNP Q02817
A	?	-	SER	deletion	UNP Q02817
A	?	-	SER	deletion	UNP Q02817
A	?	-	SER	deletion	UNP Q02817
A	?	-	THR	deletion	UNP Q02817
A	?	-	THR	deletion	UNP Q02817
A	?	-	LYS	deletion	UNP Q02817
A	?	-	ARG	deletion	UNP Q02817
A	?	-	PRO	deletion	UNP Q02817
A	?	-	ALA	deletion	UNP Q02817
A	?	-	VAL	deletion	UNP Q02817
A	?	-	THR	deletion	UNP Q02817
A	?	-	VAL	deletion	UNP Q02817

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q02817
A	?	-	GLY	deletion	UNP Q02817
A	?	-	GLY	deletion	UNP Q02817
A	?	-	GLY	deletion	UNP Q02817
A	?	-	LYS	deletion	UNP Q02817
A	?	-	THR	deletion	UNP Q02817
A	?	-	THR	deletion	UNP Q02817
A	?	-	PRO	deletion	UNP Q02817
A	?	-	HIS	deletion	UNP Q02817
A	?	-	LYS	deletion	UNP Q02817
B	?	-	PHE	deletion	UNP Q02817
B	?	-	ASP	deletion	UNP Q02817
B	?	-	PRO	deletion	UNP Q02817
B	?	-	PRO	deletion	UNP Q02817
B	?	-	ARG	deletion	UNP Q02817
B	?	-	GLN	deletion	UNP Q02817
B	?	-	GLU	deletion	UNP Q02817
B	?	-	ASN	deletion	UNP Q02817
B	?	-	GLU	deletion	UNP Q02817
B	?	-	VAL	deletion	UNP Q02817
B	?	-	ASN	deletion	UNP Q02817
B	?	-	ARG	deletion	UNP Q02817
B	?	-	GLN	deletion	UNP Q02817
B	?	-	HIS	deletion	UNP Q02817
B	?	-	SER	deletion	UNP Q02817
B	?	-	SER	deletion	UNP Q02817
B	?	-	SER	deletion	UNP Q02817
B	?	-	THR	deletion	UNP Q02817
B	?	-	THR	deletion	UNP Q02817
B	?	-	LYS	deletion	UNP Q02817
B	?	-	ARG	deletion	UNP Q02817
B	?	-	PRO	deletion	UNP Q02817
B	?	-	ALA	deletion	UNP Q02817
B	?	-	VAL	deletion	UNP Q02817
B	?	-	THR	deletion	UNP Q02817
B	?	-	VAL	deletion	UNP Q02817
B	?	-	PRO	deletion	UNP Q02817
B	?	-	GLY	deletion	UNP Q02817
B	?	-	GLY	deletion	UNP Q02817
B	?	-	GLY	deletion	UNP Q02817
B	?	-	LYS	deletion	UNP Q02817
B	?	-	THR	deletion	UNP Q02817

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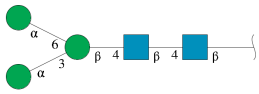
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q02817
B	?	-	PRO	deletion	UNP Q02817
B	?	-	HIS	deletion	UNP Q02817
B	?	-	LYS	deletion	UNP Q02817

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

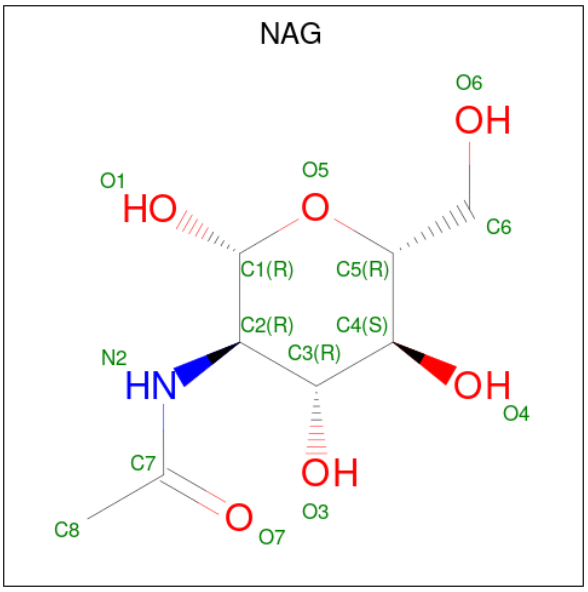


Mol	Chain	Residues	Atoms	AltConf	Trace
2	C	5	Total C N O 61 34 2 25	0	0
2	D	5	Total C N O 61 34 2 25	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Ca 1 1	0
3	B	1	Total Ca 1 1	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



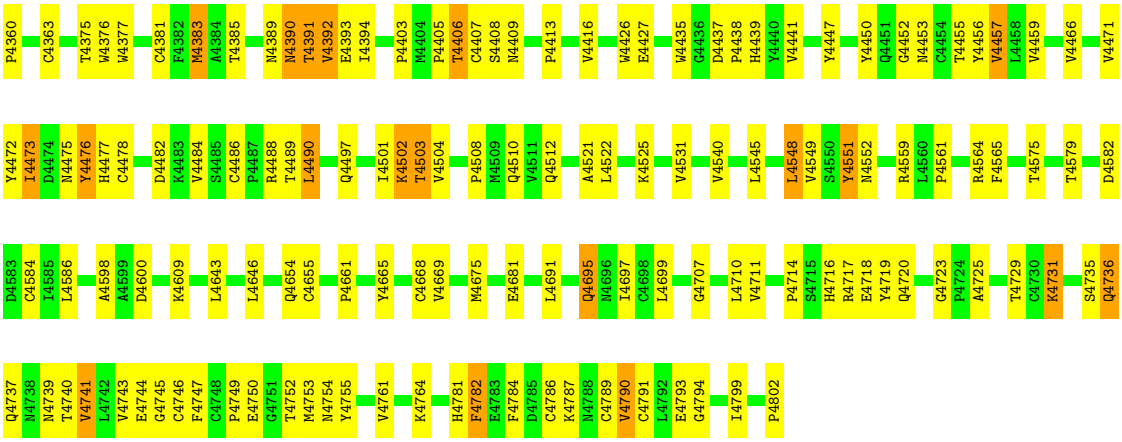
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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.

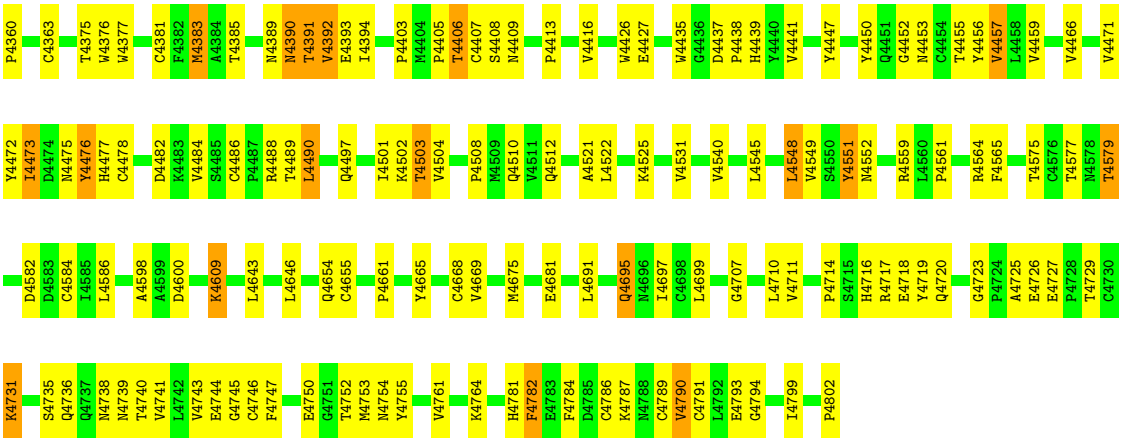
• Molecule 1: Mucin-2

Chain A:



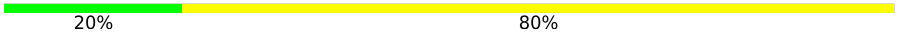
• Molecule 1: Mucin-2

Chain B:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	414056	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	79	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.671	Depositor
Minimum map value	-0.359	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.043	Depositor
Map size (Å)	371.52002, 371.52002, 371.52002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8600001, 0.8600001, 0.8600001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, BMA, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.42	0/3194	0.68	2/4371 (0.0%)
1	B	0.42	0/3194	0.67	1/4371 (0.0%)
All	All	0.42	0/6388	0.68	3/8742 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	4655	CYS	CB-CA-C	-6.21	97.98	110.40
1	A	4655	CYS	CB-CA-C	-6.21	97.99	110.40
1	A	4741	VAL	N-CA-C	-5.75	95.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3104	0	2811	95	0
1	B	3104	0	2811	96	0
2	C	61	0	52	1	0
2	D	61	0	52	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	42	0	39	5	0
4	B	42	0	39	2	0
All	All	6416	0	5804	177	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4392:VAL:CG1	1:B:4392:VAL:HG13	1.51	1.38
1:A:4392:VAL:HG13	1:B:4392:VAL:CG1	1.53	1.36
1:B:4739:ASN:O	1:B:4740:THR:HG22	1.30	1.30
1:A:4739:ASN:O	1:A:4740:THR:HG22	1.43	1.19
1:B:4739:ASN:O	1:B:4740:THR:CG2	2.11	0.98
1:A:4739:ASN:O	1:A:4740:THR:CG2	2.19	0.91
1:A:4740:THR:HB	4:A:5204:NAG:H81	1.54	0.89
1:A:4740:THR:HB	4:A:5204:NAG:C8	2.04	0.87
1:B:4740:THR:HG23	1:B:4741:VAL:H	1.44	0.81
1:A:4394:ILE:HG22	1:B:4389:ASN:O	1.82	0.80
1:A:4794:GLY:HA3	1:B:4521:ALA:HB3	1.70	0.72
1:B:4466:VAL:HG21	1:B:4545:LEU:HD21	1.71	0.72
1:A:4394:ILE:CG2	1:B:4389:ASN:O	2.36	0.71
1:B:4413:PRO:O	1:B:4426:TRP:CZ3	2.43	0.71
1:A:4466:VAL:HG21	1:A:4545:LEU:HD21	1.71	0.71
1:B:4561:PRO:HG2	1:B:4564:ARG:HB2	1.73	0.71
1:A:4392:VAL:HG13	1:B:4392:VAL:HG13	0.75	0.71
1:A:4457:VAL:HA	1:A:4472:TYR:HD1	1.55	0.71
1:A:4561:PRO:HG2	1:A:4564:ARG:HB2	1.73	0.71
1:A:4413:PRO:O	1:A:4426:TRP:CZ3	2.43	0.70
1:B:4457:VAL:HA	1:B:4472:TYR:HD1	1.55	0.70
1:A:4716:HIS:HD2	1:A:4717:ARG:HG3	1.57	0.69
1:B:4716:HIS:HD2	1:B:4717:ARG:HG3	1.57	0.69
1:A:4740:THR:CB	4:A:5204:NAG:H81	2.23	0.68
1:A:4389:ASN:O	1:B:4394:ILE:HG22	1.94	0.67
1:A:4393:GLU:HA	1:B:4390:ASN:O	1.93	0.67
1:B:4740:THR:HG23	1:B:4741:VAL:N	2.09	0.67
1:A:4413:PRO:O	1:A:4426:TRP:HZ3	1.77	0.67
1:B:4416:VAL:HG21	1:B:4427:GLU:HB2	1.77	0.66
1:B:4413:PRO:O	1:B:4426:TRP:HZ3	1.77	0.66
1:B:4739:ASN:C	1:B:4740:THR:HG22	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4416:VAL:HG21	1:A:4427:GLU:HB2	1.77	0.65
1:B:4740:THR:CG2	1:B:4741:VAL:H	2.09	0.65
1:A:4459:VAL:HG12	1:A:4471:VAL:HB	1.78	0.65
1:A:4521:ALA:HB3	1:B:4794:GLY:HA3	1.79	0.65
1:A:4782:PHE:CD2	1:A:4789:CYS:HB2	2.33	0.63
1:A:4392:VAL:O	1:B:4391:THR:HA	1.99	0.63
1:A:4392:VAL:CG1	1:B:4392:VAL:CG1	2.39	0.63
1:A:4739:ASN:C	1:A:4740:THR:HG22	2.18	0.63
1:B:4459:VAL:HG12	1:B:4471:VAL:HB	1.78	0.63
1:B:4725:ALA:HA	1:B:4743:VAL:CG2	2.28	0.63
1:B:4782:PHE:CD2	1:B:4789:CYS:HB2	2.33	0.63
1:A:4725:ALA:HA	1:A:4743:VAL:CG2	2.28	0.62
1:A:4490:LEU:HD21	1:A:4549:VAL:HG11	1.81	0.62
1:B:4490:LEU:HD21	1:B:4549:VAL:HG11	1.81	0.62
1:A:4711:VAL:HG21	1:A:4719:TYR:HB2	1.82	0.61
1:B:4787:LYS:HA	1:B:4802:PRO:HA	1.83	0.61
1:A:4787:LYS:HA	1:A:4802:PRO:HA	1.83	0.61
1:A:4435:TRP:O	1:A:4439:HIS:HB2	2.01	0.61
1:B:4643:LEU:HD23	1:B:4681:GLU:HG2	1.82	0.60
1:A:4643:LEU:HD23	1:A:4681:GLU:HG2	1.82	0.60
1:B:4711:VAL:HG21	1:B:4719:TYR:HB2	1.82	0.60
1:B:4435:TRP:O	1:B:4439:HIS:HB2	2.01	0.60
1:B:4385:THR:HB	1:B:4393:GLU:HB2	1.84	0.59
1:B:4503:THR:HG22	1:B:4508:PRO:HG3	1.85	0.59
1:A:4718:GLU:HG3	1:A:4720:GLN:HE21	1.69	0.58
1:B:4718:GLU:HG3	1:B:4720:GLN:HE21	1.69	0.58
1:A:4503:THR:HG22	1:A:4508:PRO:HG3	1.85	0.58
1:A:4385:THR:HB	1:A:4393:GLU:HB2	1.85	0.57
1:A:4723:GLY:HA3	1:A:4747:PHE:CE2	2.39	0.57
1:A:4457:VAL:HA	1:A:4472:TYR:CD1	2.38	0.57
1:A:4551:TYR:HD1	1:A:4552:ASN:N	2.02	0.57
1:A:4389:ASN:O	1:B:4394:ILE:CG2	2.52	0.57
1:B:4723:GLY:HA3	1:B:4747:PHE:CE2	2.39	0.57
1:A:4390:ASN:O	1:B:4393:GLU:HA	2.04	0.57
1:B:4551:TYR:HD1	1:B:4552:ASN:N	2.02	0.57
1:A:4740:THR:HB	4:A:5204:NAG:H82	1.84	0.56
1:A:4740:THR:HG23	1:A:4741:VAL:N	2.20	0.56
1:B:4457:VAL:HA	1:B:4472:TYR:CD1	2.38	0.56
1:A:4584:CYS:HB3	1:A:4598:ALA:HB3	1.88	0.56
1:B:4385:THR:N	1:B:4393:GLU:O	2.32	0.56
1:B:4476:TYR:HD2	1:B:4482:ASP:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4584:CYS:HB3	1:B:4598:ALA:HB3	1.88	0.56
1:B:4740:THR:HB	4:B:5204:NAG:H82	1.88	0.56
1:B:4450:TYR:OH	1:B:4600:ASP:OD1	2.23	0.55
1:A:4385:THR:N	1:A:4393:GLU:O	2.32	0.55
1:B:4545:LEU:HD23	1:B:4565:PHE:HZ	1.71	0.55
1:B:4725:ALA:HA	1:B:4743:VAL:HG21	1.89	0.55
1:A:4476:TYR:HD2	1:A:4482:ASP:HA	1.71	0.55
1:B:4782:PHE:N	1:B:4782:PHE:CD1	2.75	0.55
1:A:4545:LEU:HD23	1:A:4565:PHE:HZ	1.71	0.54
1:A:4782:PHE:CD1	1:A:4782:PHE:N	2.75	0.54
1:B:4752:THR:HG22	1:B:4764:LYS:HG2	1.90	0.54
1:A:4752:THR:HG22	1:A:4764:LYS:HG2	1.90	0.53
1:A:4725:ALA:HA	1:A:4743:VAL:HG21	1.89	0.53
1:B:4403:PRO:HA	1:B:4426:TRP:NE1	2.24	0.53
1:B:4714:PRO:HG2	1:B:4716:HIS:CE1	2.45	0.52
1:A:4403:PRO:HA	1:A:4426:TRP:NE1	2.24	0.52
1:A:4714:PRO:HG2	1:A:4716:HIS:CE1	2.45	0.51
1:B:4405:PRO:HA	1:B:4413:PRO:HG3	1.91	0.51
1:A:4450:TYR:OH	1:A:4600:ASP:OD1	2.23	0.51
1:B:4453:ASN:HB2	1:B:4476:TYR:CD1	2.45	0.51
1:A:4405:PRO:HA	1:A:4413:PRO:HG3	1.92	0.51
1:B:4497:GLN:HG2	1:B:4512:GLN:HE21	1.76	0.51
1:A:4725:ALA:HA	1:A:4743:VAL:HG22	1.91	0.51
1:B:4725:ALA:HA	1:B:4743:VAL:HG22	1.91	0.51
1:A:4453:ASN:HB2	1:A:4476:TYR:CD1	2.46	0.50
1:A:4497:GLN:HG2	1:A:4512:GLN:HE21	1.76	0.50
1:B:4531:VAL:HG22	1:B:4540:VAL:HG22	1.95	0.49
1:A:4545:LEU:HD23	1:A:4565:PHE:CZ	2.48	0.49
1:A:4707:GLY:HA2	1:A:4710:LEU:HD11	1.94	0.49
1:A:4781:HIS:CE1	1:A:4790:VAL:HB	2.48	0.49
1:A:4391:THR:HA	1:B:4392:VAL:O	2.13	0.49
1:B:4545:LEU:HD23	1:B:4565:PHE:CZ	2.48	0.49
1:A:4437:ASP:HB3	1:A:4438:PRO:HD3	1.95	0.48
1:A:4531:VAL:HG22	1:A:4540:VAL:HG22	1.95	0.48
1:B:4437:ASP:HB3	1:B:4438:PRO:HD3	1.95	0.48
1:B:4781:HIS:CE1	1:B:4790:VAL:HB	2.48	0.48
1:B:4761:VAL:HG23	1:B:4761:VAL:O	2.14	0.48
1:B:4707:GLY:HA2	1:B:4710:LEU:HD11	1.94	0.48
1:A:4761:VAL:HG23	1:A:4761:VAL:O	2.14	0.48
1:B:4473:ILE:HD12	1:B:4473:ILE:HA	1.73	0.47
1:B:4719:TYR:HA	1:B:4745:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4740:THR:HB	4:B:5204:NAG:C8	2.44	0.47
1:A:4711:VAL:HG21	1:A:4719:TYR:CD1	2.49	0.47
1:B:4711:VAL:HG21	1:B:4719:TYR:CD1	2.50	0.47
1:A:4719:TYR:HA	1:A:4745:GLY:O	2.14	0.47
1:B:4729:THR:HG22	1:B:4754:ASN:HB3	1.96	0.47
1:A:4729:THR:HG22	1:A:4754:ASN:HB3	1.96	0.46
1:A:4643:LEU:HA	1:A:4646:LEU:HD13	1.98	0.46
1:A:4665:TYR:O	1:A:4669:VAL:HG23	2.16	0.46
1:B:4754:ASN:OD1	1:B:4755:TYR:N	2.49	0.46
1:A:4548:LEU:HB3	1:A:4559:ARG:HB3	1.98	0.45
1:B:4643:LEU:HA	1:B:4646:LEU:HD13	1.98	0.45
1:A:4731:LYS:HA	1:A:4731:LYS:HD3	1.53	0.45
1:B:4548:LEU:HB3	1:B:4559:ARG:HB3	1.98	0.45
1:A:4406:THR:HG21	2:C:2:NAG:O7	2.17	0.45
1:A:4510:GLN:NE2	1:A:4522:LEU:HA	2.31	0.45
1:B:4510:GLN:NE2	1:B:4522:LEU:HA	2.31	0.45
1:B:4665:TYR:O	1:B:4669:VAL:HG23	2.16	0.45
1:A:4416:VAL:CG2	1:A:4427:GLU:HB2	2.45	0.45
1:B:4731:LYS:HD3	1:B:4731:LYS:HA	1.53	0.45
1:A:4754:ASN:OD1	1:A:4755:TYR:N	2.49	0.45
1:A:4452:GLY:HA3	1:A:4456:TYR:HE2	1.83	0.44
1:B:4406:THR:HG21	2:D:2:NAG:O7	2.17	0.44
1:B:4490:LEU:HD21	1:B:4549:VAL:CG1	2.46	0.44
1:A:4740:THR:CG2	1:A:4741:VAL:N	2.81	0.44
1:B:4393:GLU:N	1:B:4393:GLU:OE1	2.50	0.44
1:B:4714:PRO:HG2	1:B:4716:HIS:NE2	2.33	0.44
1:A:4393:GLU:OE1	1:A:4393:GLU:N	2.50	0.44
1:A:4740:THR:CB	4:A:5204:NAG:C8	2.85	0.44
1:A:4575:THR:OG1	1:A:4582:ASP:O	2.34	0.44
1:A:4473:ILE:HD12	1:A:4473:ILE:HA	1.73	0.43
1:B:4452:GLY:HA3	1:B:4456:TYR:HE2	1.83	0.43
1:B:4377:TRP:HE1	1:B:4381:CYS:HA	1.84	0.43
1:A:4441:VAL:HG12	1:A:4447:TYR:HB2	2.01	0.43
1:B:4416:VAL:CG2	1:B:4427:GLU:HB2	2.45	0.43
1:A:4363:CYS:HB3	1:A:4376:TRP:CE3	2.53	0.43
1:A:4668:CYS:SG	1:A:4681:GLU:HB2	2.59	0.43
1:B:4363:CYS:HB3	1:B:4376:TRP:CE3	2.53	0.43
1:B:4740:THR:CG2	1:B:4741:VAL:N	2.73	0.43
1:A:4377:TRP:HE1	1:A:4381:CYS:HA	1.84	0.43
1:A:4714:PRO:HG2	1:A:4716:HIS:NE2	2.33	0.43
1:B:4668:CYS:SG	1:B:4681:GLU:HB2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4490:LEU:HD21	1:A:4549:VAL:CG1	2.46	0.42
1:A:4502:LYS:HB3	1:A:4502:LYS:HE3	1.37	0.42
1:B:4577:THR:O	1:B:4579:THR:N	2.46	0.42
1:B:4718:GLU:O	1:B:4720:GLN:HG3	2.19	0.42
1:B:4441:VAL:HG12	1:B:4447:TYR:HB2	2.00	0.42
1:B:4383:MET:O	1:B:4394:ILE:HG13	2.19	0.42
1:B:4609:LYS:HE2	1:B:4609:LYS:HB3	1.81	0.42
1:A:4718:GLU:O	1:A:4720:GLN:HG3	2.19	0.42
1:B:4497:GLN:HG2	1:B:4512:GLN:NE2	2.35	0.42
1:A:4695:GLN:H	1:A:4695:GLN:HG2	1.51	0.41
1:B:4695:GLN:H	1:B:4695:GLN:HG2	1.51	0.41
1:A:4383:MET:O	1:A:4394:ILE:HG13	2.20	0.41
1:A:4718:GLU:O	1:A:4746:CYS:HA	2.21	0.41
1:A:4736:GLN:O	1:A:4737:GLN:C	2.60	0.41
1:B:4575:THR:OG1	1:B:4582:ASP:O	2.33	0.41
1:B:4718:GLU:O	1:B:4746:CYS:HA	2.21	0.41
1:B:4738:ASN:OD1	1:B:4738:ASN:N	2.53	0.41
1:A:4497:GLN:HG2	1:A:4512:GLN:NE2	2.35	0.40
1:A:4717:ARG:HH22	1:A:4754:ASN:ND2	2.20	0.40
1:B:4738:ASN:OD1	1:B:4738:ASN:O	2.39	0.40
1:B:4717:ARG:HH22	1:B:4754:ASN:ND2	2.20	0.40
1:B:4726:GLU:O	1:B:4727:GLU:C	2.60	0.40
1:A:4749:PRO:HD2	1:A:4752:THR:OG1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/407 (98%)	363 (91%)	35 (9%)	1 (0%)	41	72
1	B	399/407 (98%)	363 (91%)	35 (9%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	798/814 (98%)	726 (91%)	70 (9%)	2 (0%)	44 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4661	PRO
1	B	4661	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	351/362 (97%)	300 (86%)	51 (14%)	3 12
1	B	351/362 (97%)	300 (86%)	51 (14%)	3 12
All	All	702/724 (97%)	600 (86%)	102 (14%)	6 12

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4360	PRO
1	A	4375	THR
1	A	4383	MET
1	A	4390	ASN
1	A	4391	THR
1	A	4392	VAL
1	A	4406	THR
1	A	4407	CYS
1	A	4408	SER
1	A	4409	ASN
1	A	4455	THR
1	A	4457	VAL
1	A	4473	ILE
1	A	4475	ASN
1	A	4476	TYR
1	A	4477	HIS

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Mol	Chain	Res	Type
1	A	4478	CYS
1	A	4484	VAL
1	A	4486	CYS
1	A	4488	ARG
1	A	4489	THR
1	A	4490	LEU
1	A	4501	ILE
1	A	4502	LYS
1	A	4503	THR
1	A	4504	VAL
1	A	4525	LYS
1	A	4548	LEU
1	A	4551	TYR
1	A	4579	THR
1	A	4586	LEU
1	A	4609	LYS
1	A	4654	GLN
1	A	4675	MET
1	A	4691	LEU
1	A	4695	GLN
1	A	4697	ILE
1	A	4699	LEU
1	A	4731	LYS
1	A	4735	SER
1	A	4736	GLN
1	A	4744	GLU
1	A	4750	GLU
1	A	4753	MET
1	A	4782	PHE
1	A	4784	PHE
1	A	4786	CYS
1	A	4790	VAL
1	A	4791	CYS
1	A	4793	GLU
1	A	4799	ILE
1	B	4360	PRO
1	B	4375	THR
1	B	4383	MET
1	B	4390	ASN
1	B	4391	THR
1	B	4392	VAL
1	B	4406	THR

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Mol	Chain	Res	Type
1	B	4407	CYS
1	B	4408	SER
1	B	4409	ASN
1	B	4455	THR
1	B	4457	VAL
1	B	4473	ILE
1	B	4475	ASN
1	B	4476	TYR
1	B	4477	HIS
1	B	4478	CYS
1	B	4484	VAL
1	B	4486	CYS
1	B	4488	ARG
1	B	4489	THR
1	B	4490	LEU
1	B	4501	ILE
1	B	4502	LYS
1	B	4503	THR
1	B	4504	VAL
1	B	4525	LYS
1	B	4548	LEU
1	B	4551	TYR
1	B	4579	THR
1	B	4586	LEU
1	B	4609	LYS
1	B	4654	GLN
1	B	4675	MET
1	B	4691	LEU
1	B	4695	GLN
1	B	4697	ILE
1	B	4699	LEU
1	B	4731	LYS
1	B	4735	SER
1	B	4736	GLN
1	B	4744	GLU
1	B	4750	GLU
1	B	4753	MET
1	B	4782	PHE
1	B	4784	PHE
1	B	4786	CYS
1	B	4790	VAL
1	B	4791	CYS

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Mol	Chain	Res	Type
1	B	4793	GLU
1	B	4799	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4716	HIS
1	A	4720	GLN
1	B	4716	HIS
1	B	4720	GLN
1	B	4781	HIS

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

10 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	NAG	C	1	1,2	14,14,15	0.34	0	17,19,21	0.95	1 (5%)
2	NAG	C	2	2	14,14,15	0.35	0	17,19,21	0.80	0
2	BMA	C	3	2	11,11,12	0.58	0	15,15,17	2.46	2 (13%)
2	MAN	C	4	2	11,11,12	0.56	0	15,15,17	3.34	4 (26%)
2	MAN	C	5	2	11,11,12	0.24	0	15,15,17	0.79	0
2	NAG	D	1	1,2	14,14,15	0.34	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	D	3	2	11,11,12	0.60	0	15,15,17	2.47	2 (13%)
2	MAN	D	4	2	11,11,12	0.59	0	15,15,17	3.33	4 (26%)
2	MAN	D	5	2	11,11,12	0.25	0	15,15,17	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	BMA	O2-C2-C3	8.56	127.29	110.14
2	C	3	BMA	O2-C2-C3	8.55	127.26	110.14
2	C	4	MAN	O2-C2-C3	8.06	126.29	110.14
2	D	4	MAN	O2-C2-C3	8.04	126.25	110.14
2	C	4	MAN	O3-C3-C4	-5.94	96.61	110.35
2	D	4	MAN	O3-C3-C4	-5.94	96.62	110.35
2	D	4	MAN	O4-C4-C5	-5.73	95.07	109.30
2	C	4	MAN	O4-C4-C5	-5.72	95.08	109.30
2	C	4	MAN	O5-C5-C6	-5.08	99.24	107.20
2	D	4	MAN	O5-C5-C6	-5.03	99.31	107.20
2	D	3	BMA	C2-C3-C4	2.39	115.04	110.89
2	C	3	BMA	C2-C3-C4	2.37	115.00	110.89
2	D	1	NAG	C1-C2-N2	-2.23	106.67	110.49
2	C	1	NAG	C1-C2-N2	-2.21	106.72	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C3-C2-N2-C7
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	5	MAN	C4-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6

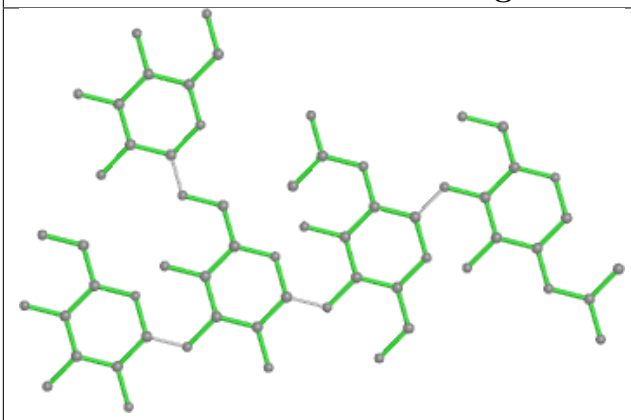
There are no ring outliers.

2 monomers are involved in 2 short contacts:

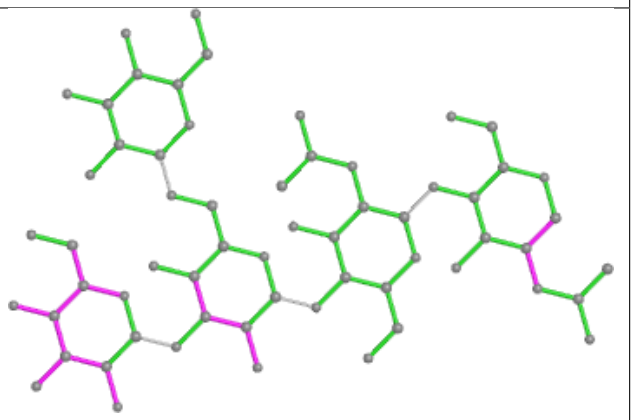
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	C	2	NAG	1	0

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

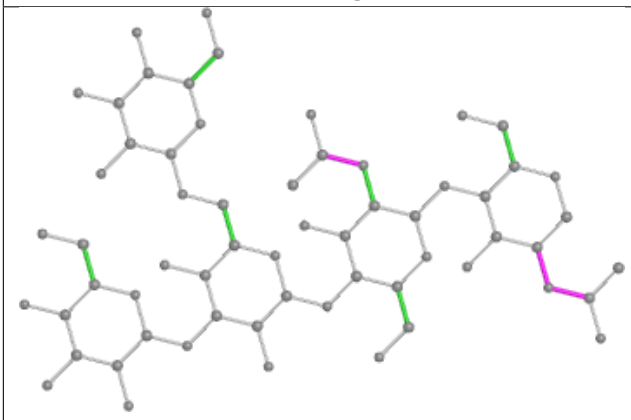
Oligosaccharide Chain C



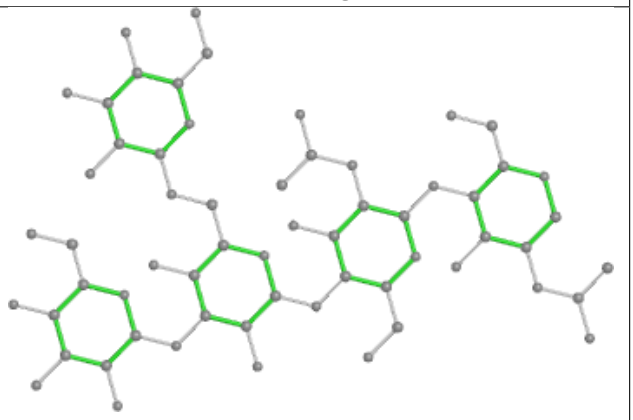
Bond lengths



Bond angles

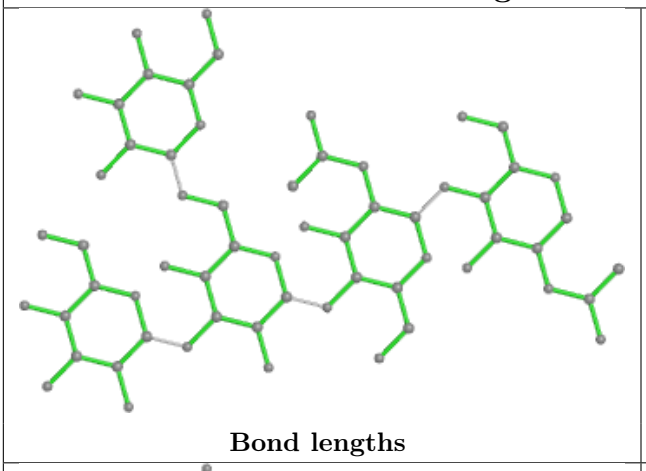


Torsions

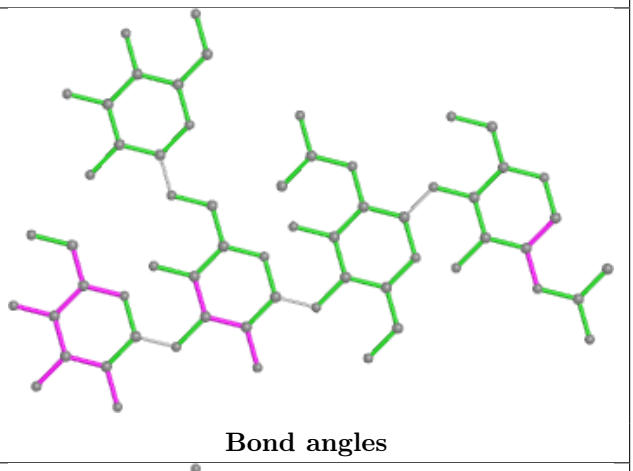


Rings

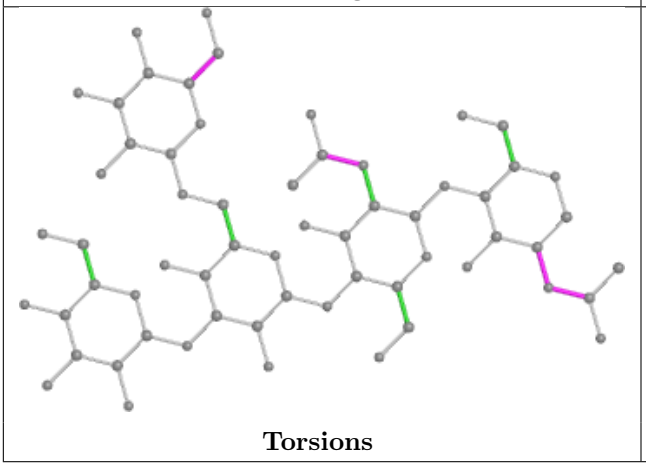
Oligosaccharide Chain D



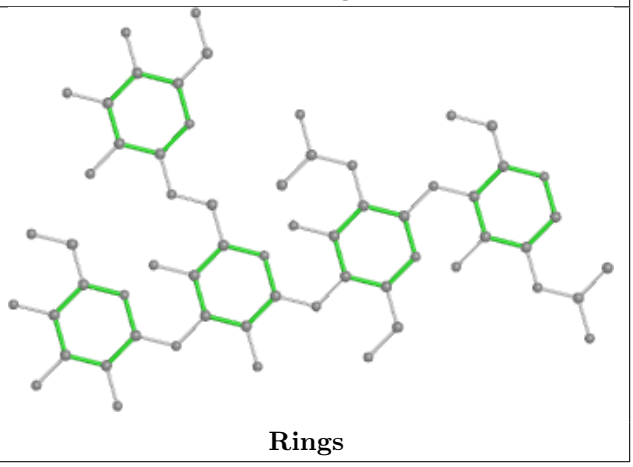
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAG	B	5204	1	14,14,15	0.39	0	17,19,21	0.81	0
4	NAG	B	5203	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	5204	1	14,14,15	0.39	0	17,19,21	0.81	0
4	NAG	A	5202	-	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	A	5203	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	B	5202	-	14,14,15	0.23	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	5204	1	-	0/6/23/26	0/1/1/1
4	NAG	B	5203	1	-	2/6/23/26	0/1/1/1
4	NAG	A	5204	1	-	0/6/23/26	0/1/1/1
4	NAG	A	5202	-	-	0/6/23/26	0/1/1/1
4	NAG	A	5203	1	-	2/6/23/26	0/1/1/1
4	NAG	B	5202	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5203	NAG	C8-C7-N2-C2
4	A	5203	NAG	O7-C7-N2-C2
4	B	5203	NAG	C8-C7-N2-C2
4	B	5203	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5204	NAG	2	0
4	A	5204	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4613:PRO	C	4637:ASP	N	39.48
1	B	4613:PRO	C	4637:ASP	N	39.48
1	A	4365:ASP	C	4375:THR	N	12.03
1	B	4365:ASP	C	4375:THR	N	12.03
1	A	4513:VAL	C	4518:GLN	N	3.13
1	B	4513:VAL	C	4518:GLN	N	3.13

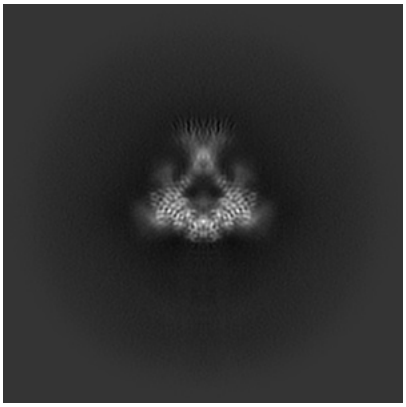
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13897. These allow visual inspection of the internal detail of the map and identification of artifacts.

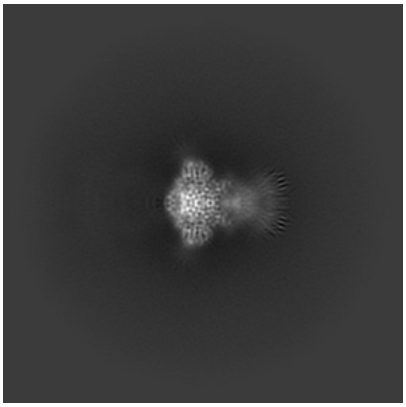
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

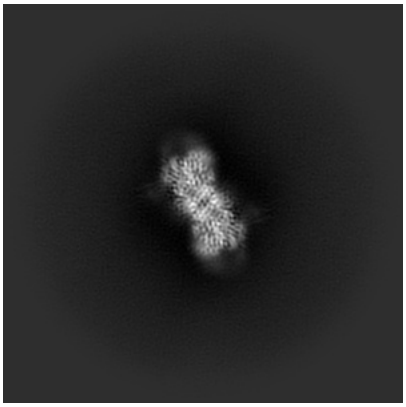
6.1.1 Primary map



X



Y



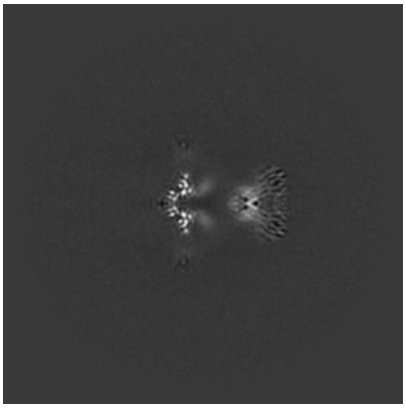
Z

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

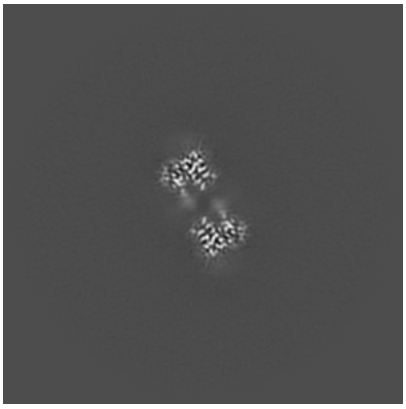
6.2 Central slices

6.2.1 Primary map

X Index: 216



Y Index: 216

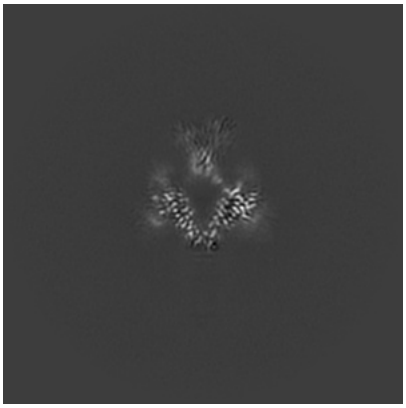


Z Index: 216

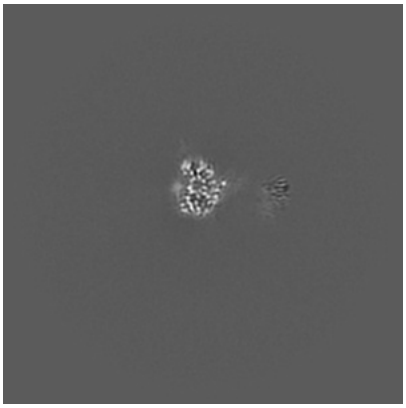
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

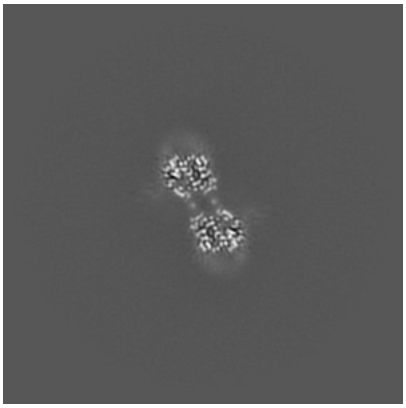
6.3.1 Primary map



X Index: 213



Y Index: 188

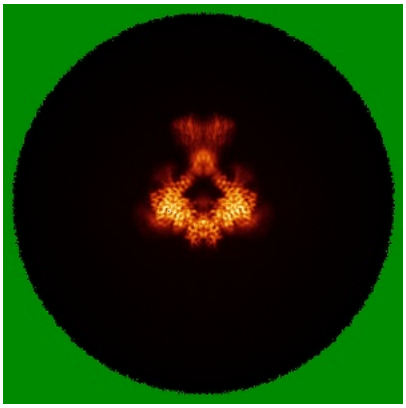


Z Index: 207

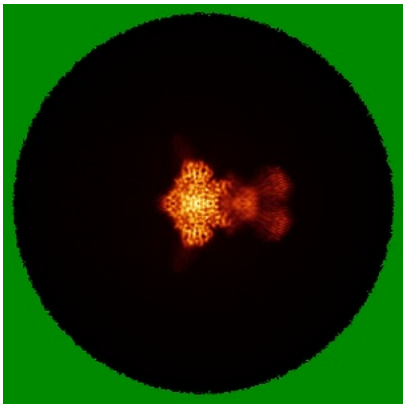
The images above show the largest variance slices of the map in three orthogonal directions.

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

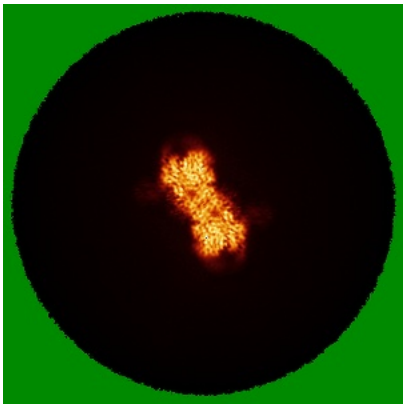
6.4.1 Primary map



X



Y

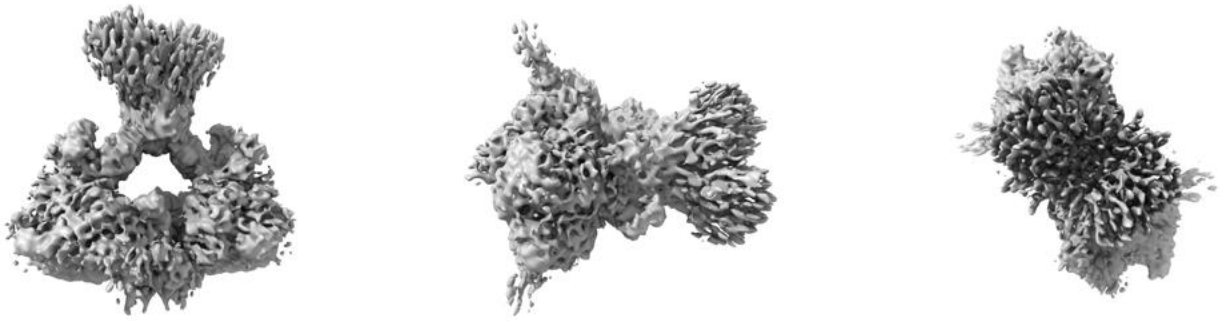


Z

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 0.043. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

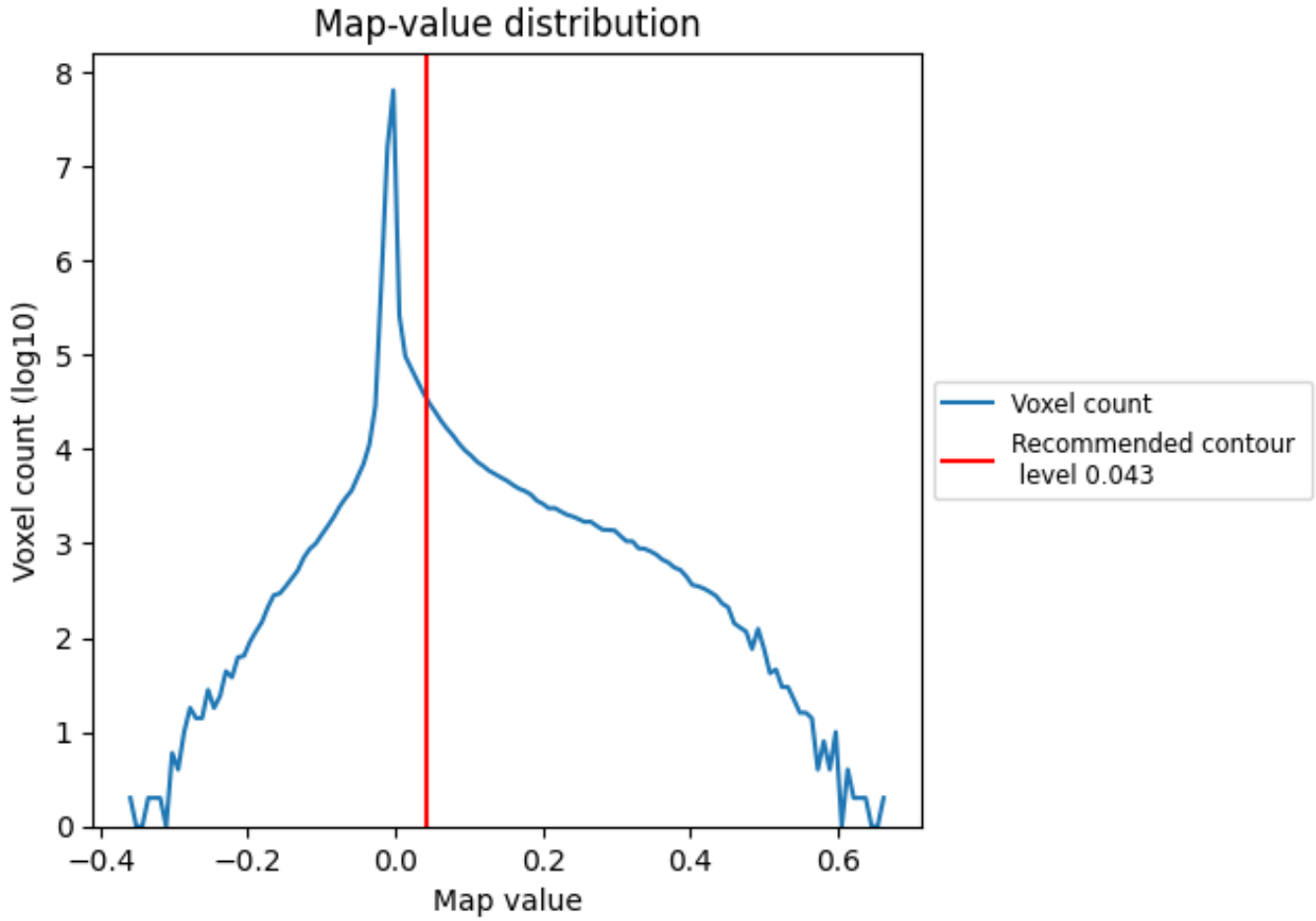
6.6 Mask visualisation (i)

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

7 Map analysis

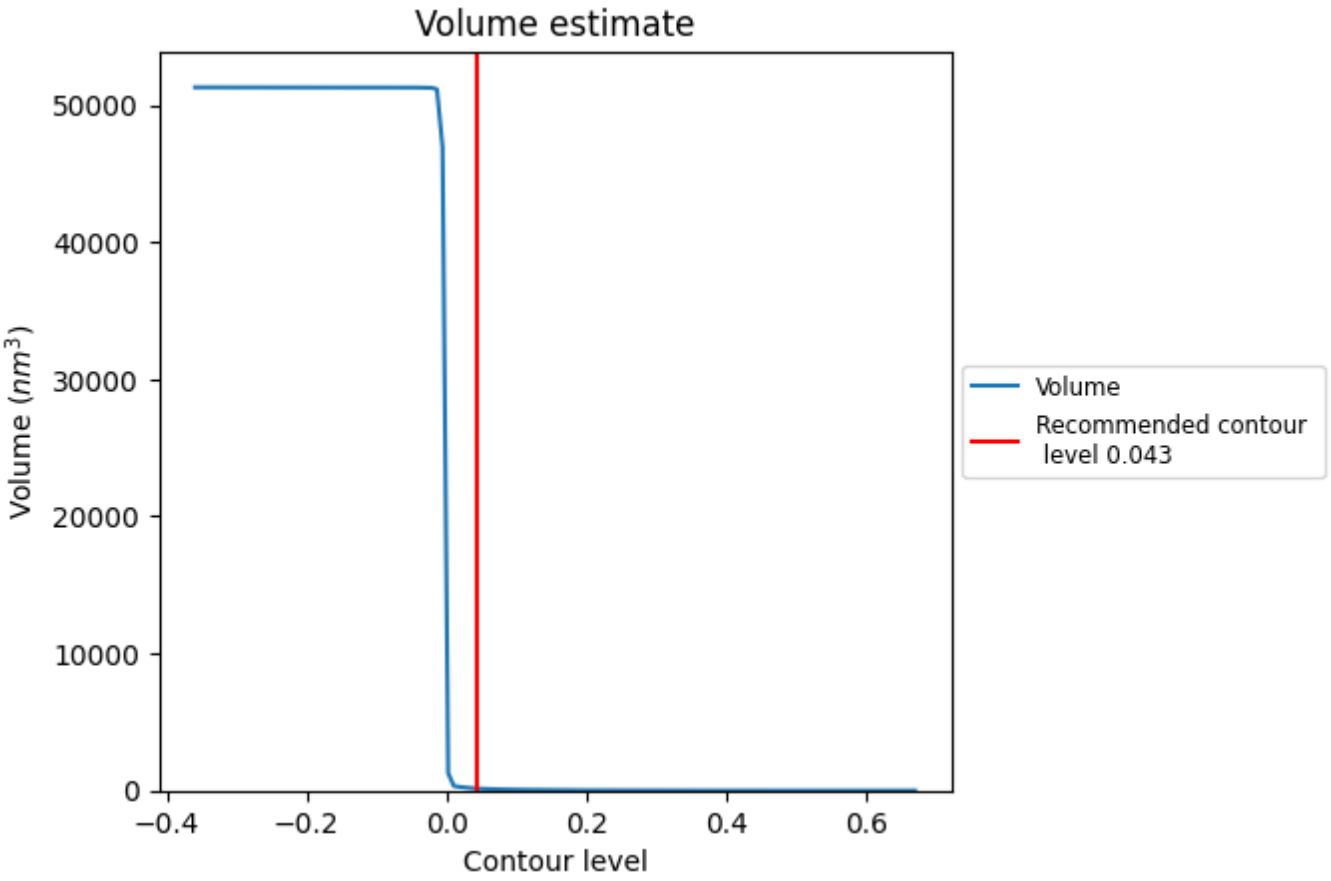
This section contains the results of statistical analysis of the map.

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.

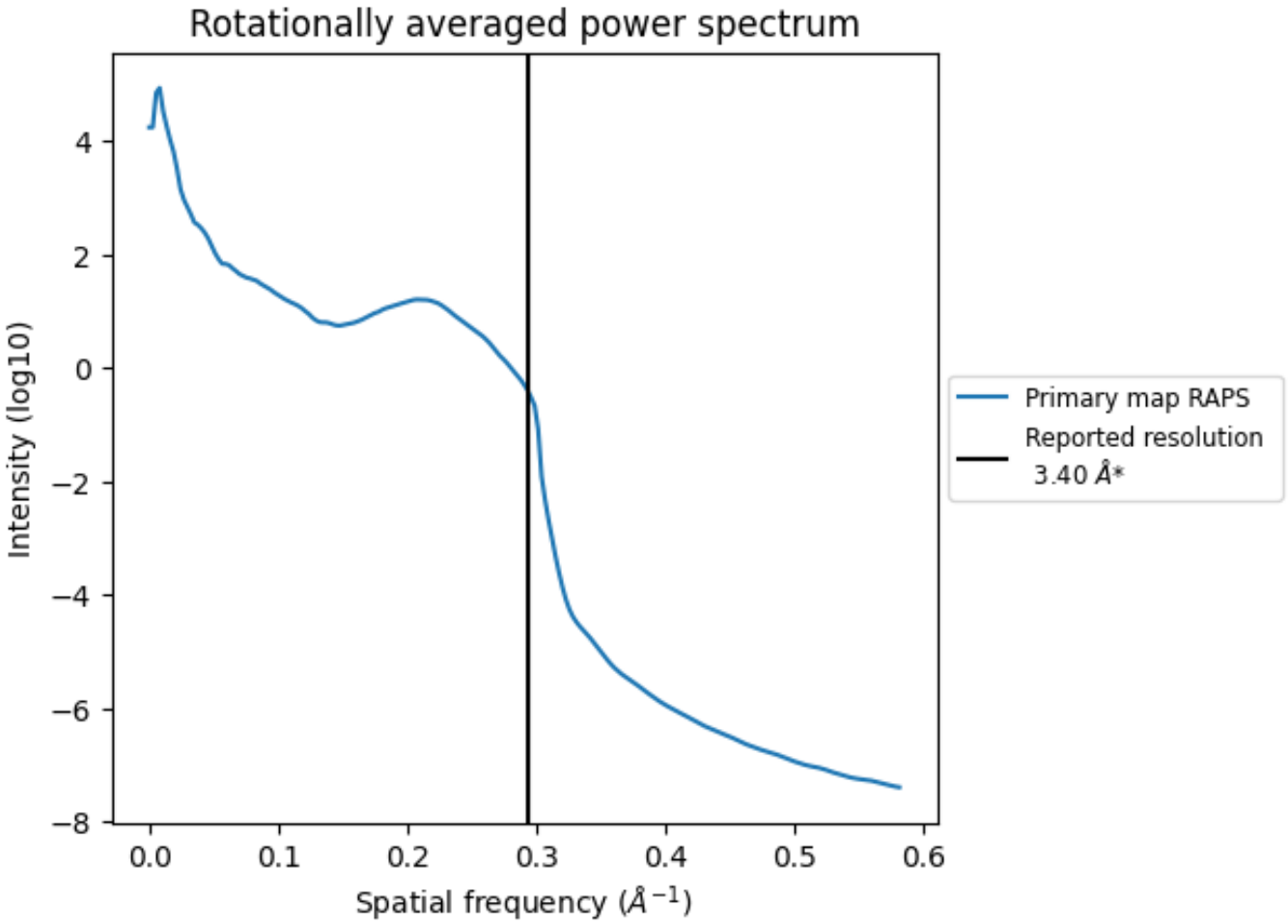
7.2 Volume estimate



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 137 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}

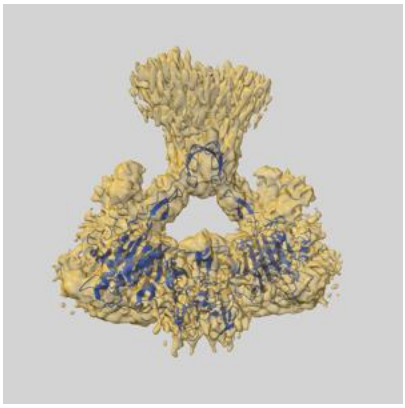
8 Fourier-Shell correlation (i)

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

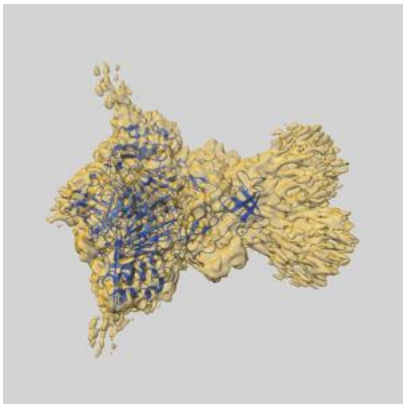
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13897 and PDB model 7QCN. Per-residue inclusion information can be found in section 3 on page 7.

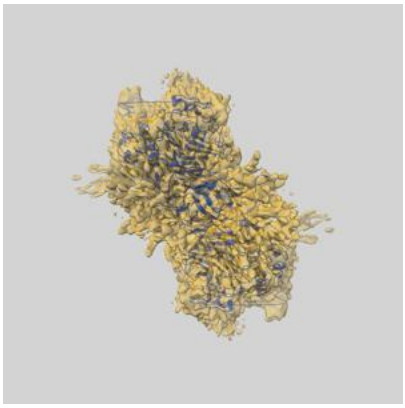
9.1 Map-model overlay



X



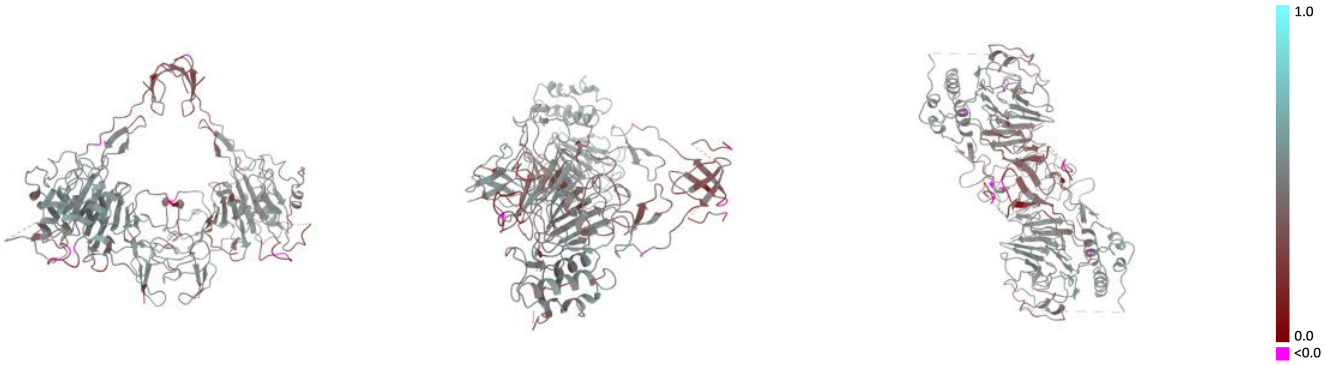
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.043 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.

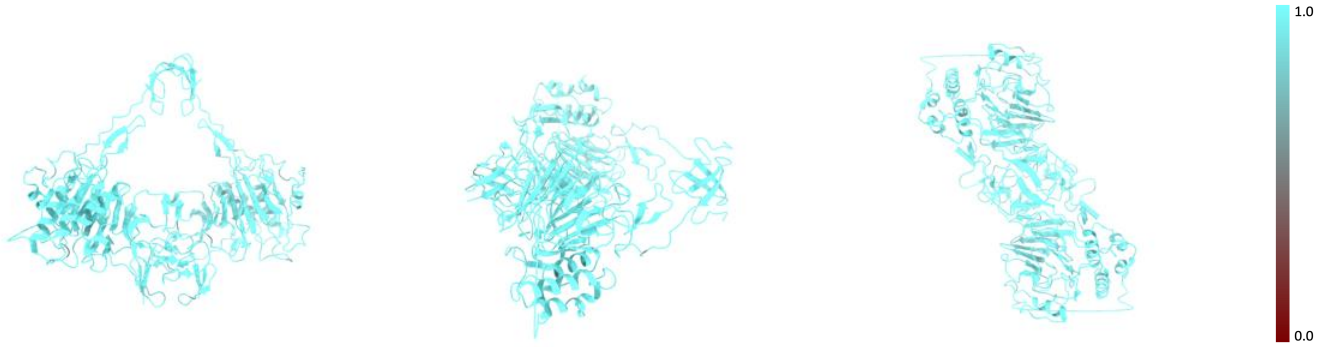
9.2 Q-score mapped to coordinate model



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.

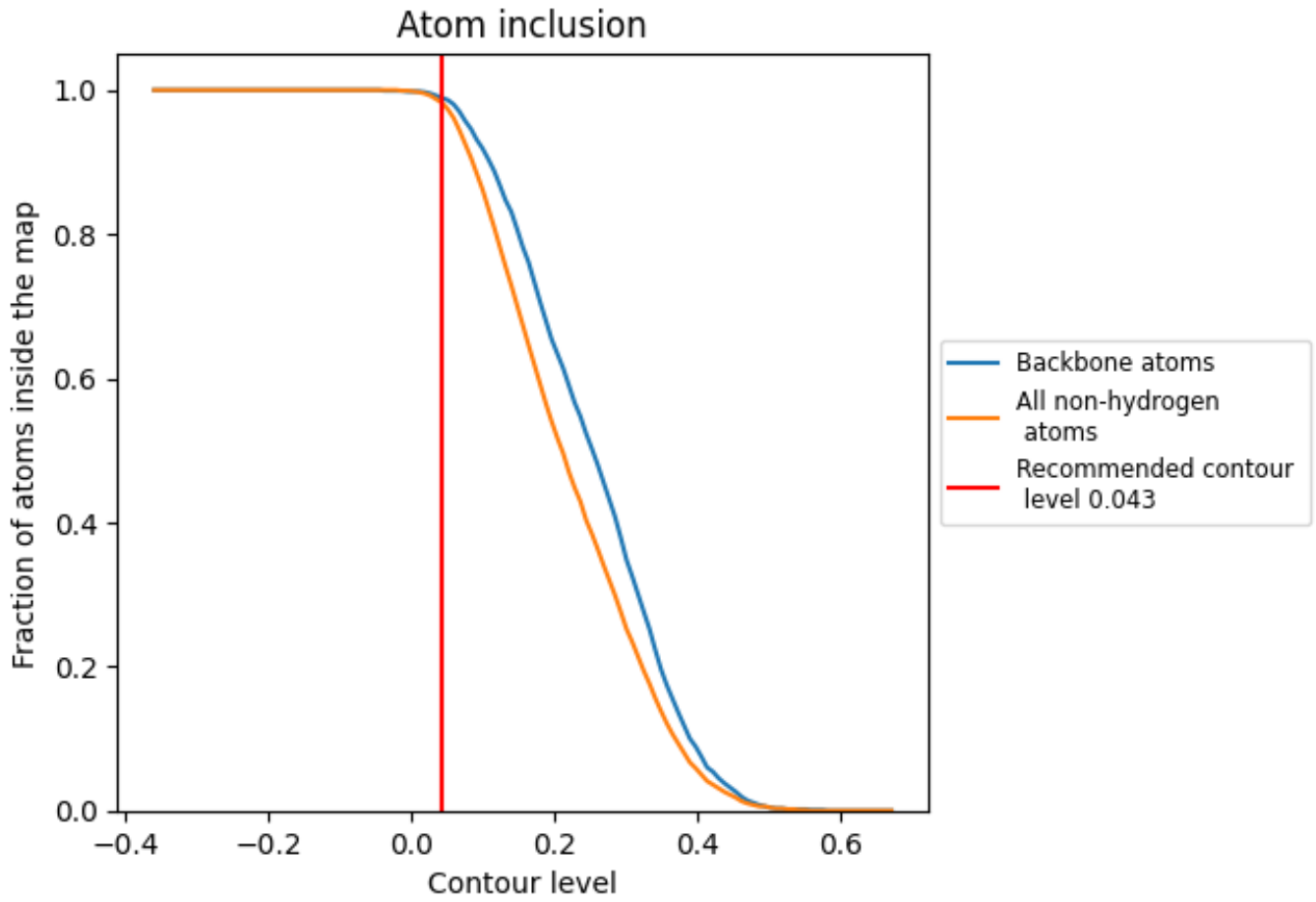
9.3 Atom inclusion mapped to coordinate model



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 (0.043).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.043) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.4380
A	0.9800	0.4290
B	0.9830	0.4500
C	0.9670	0.4020
D	0.9670	0.3750