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PDB ID	:	7CN9
EMDB ID	:	EMD-30419
Title	:	Cryo-EM structure of SARS-CoV-2 Spike ectodomain
Authors	:	Ho, M.; Chang, Y.; Wang, C.; Wu, Y.; Huang, H.; Chen, T.; Lo, J.M.; Chen,
		X.; Ma, C.
Deposited on	:	2020-07-30
Resolution	:	4.70 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 (i) 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 (1)) were used in the production of this report:

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.70 Å.

Sidechain outliers

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	Percentile Ran	ks Value				
Ramachandran outliers	1.1%					
Sidechain outliers		2.7%				
Worse	Worse					
Percenti	le relative to all structures					
🛛 Percenti	le relative to all EM structures					
	Whole archive	EM structures				
Metric	$(\# {\rm Entries})$	(# Entries)				
Ramachandran outliers	154571	4023				

154315

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

3826

Mol	Chain	Length	Quality of chain	
1	А	1127	44% 87%	• 10%
1	В	1127	37%	• 10%
1	С	1127	39%	• 8%
2	Е	2	50%	
2	Н	2	50%	
2	Ν	2	50%	
2	W	2	100%	
2	Х	2	50%	
2	Z	2	100% 50% 50%	



				<u> </u>						
NIO	Chain	Length	Qualit	Quality of chain						
			50%							
2	d	2	50%	50%						
2	f	2	50%	50%						
			67%							
3	k	3	33%	67%						
			67%							
4	V	3		100%						
			33%							
4	р	3		100%						
				100%						
5	h	4	50%	50%						
			75%							
6	Q	4		100%						



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24052 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Δ	1011	Total	С	Ν	Ο	\mathbf{S}	0	0
	1011	7727	4935	1292	1465	35	0	0	
1	В	1010	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	1010	7674	4895	1285	1458	36	0	0	
1 C	1027	Total	С	Ν	Ο	\mathbf{S}	0	0	
	U	1057	7889	5040	1316	1498	35	0	0

• Molecule 1 is a protein called Spike glycoprotein.

	There are 15	discrepancies	between	the modelled	and	reference	sequences:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	682	GLY	ARG	engineered mutation	UNP P0DTC2
А	683	SER	ARG	engineered mutation	UNP P0DTC2
А	685	GLY	ARG	engineered mutation	UNP P0DTC2
А	986	PRO	LYS	engineered mutation	UNP P0DTC2
А	987	PRO	VAL	engineered mutation	UNP P0DTC2
В	682	GLY	ARG	engineered mutation	UNP P0DTC2
В	683	SER	ARG	engineered mutation	UNP P0DTC2
В	685	GLY	ARG	engineered mutation	UNP P0DTC2
В	986	PRO	LYS	engineered mutation	UNP P0DTC2
В	987	PRO	VAL	engineered mutation	UNP P0DTC2
С	682	GLY	ARG	engineered mutation	UNP P0DTC2
С	683	SER	ARG	engineered mutation	UNP P0DTC2
С	685	GLY	ARG	engineered mutation	UNP P0DTC2
С	986	PRO	LYS	engineered mutation	UNP P0DTC2
С	987	PRO	VAL	engineered mutation	UNP P0DTC2

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms	AltConf	Trace
2	Е	2	Total C N O 28 16 2 10	0	0
2	Х	2	Total C N O 28 16 2 10	0	0
2	W	2	Total C N O 28 16 2 10	0	0
2	Ζ	2	Total C N O 28 16 2 10	0	0
2	d	2	Total C N O 28 16 2 10	0	0
2	f	2	Total C N O 28 16 2 10	0	0
2	Н	2	Total C N O 28 16 2 10	0	0
2	Ν	2	Total C N O 28 16 2 10	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[al pha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	k	3	Total 38	C 22	N 2	0 14	0	0

• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
4	р	3	Total C N O 39 22 2 15	0	0
4	V	3	Total C N O 39 22 2 15	0	0

 $\bullet \ \ Molecule \ 5 \ is \ an \ oligosaccharide \ called \ alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac$



pyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	h	4	Total 50	C 28	N 2	O 20	0	0

• Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
6	Q	4	Total 50	C 28	N 2	O 20	0	0

• Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms			AltConf	
7	А	1	Total 98	C 56	N 7	O 35	0



Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
7	٨	1	Total	С	Ν	0	0
(А	1	98	56	7	35	0
7	٨	1	Total	С	Ν	0	0
1	A	1	98	56	7	35	0
7	٨	1	Total	С	Ν	0	0
1	A	1	98	56	7	35	0
7	٨	1	Total	С	Ν	0	0
1	A	1	98	56	7	35	0
7	٨	1	Total	С	Ν	0	0
(А	1	98	56	7	35	0
7	٨	1	Total	С	Ν	0	0
(А	1	98	56	7	35	0
7	D	1	Total	С	Ν	0	0
(D	1	126	72	9	45	0
7	D	1	Total	С	Ν	0	0
(В	1	126	72	9	45	0
7	р	1	Total	С	Ν	0	0
(В	1	126	72	9	45	0
7	р	1	Total	С	Ν	0	0
(В	1	126	72	9	45	0
	D	1	Total	С	Ν	0	0
(В	1	126	72	9	45	0
7	р	1	Total	С	Ν	0	0
(В	1	126	72	9	45	0
7	р	1	Total	С	Ν	0	0
(D	1	126	72	9	45	0
7	D	1	Total	С	Ν	0	0
1	D	1	126	72	9	45	0
7	D	1	Total	С	Ν	0	0
(D	1	126	72	9	45	0
7	C	1	Total	С	Ν	0	0
1	U	1	98	56	7	35	0
7	С	1	Total	С	Ν	0	0
1	U	1	98	56	7	35	0
7	C	1	Total	С	Ν	0	0
'		L	98	56	7	35	U
7	С	1	Total	С	Ν	Ο	0
(⁽		1	98	56	7	35	U
7	С	1	Total	С	Ν	Ο	0
(1	98	56	7	35	U
7	C	1	Total	С	Ν	0	0
(U	1	98	56	7	35	U



Mol	Chain	Residues	Atoms			AltConf	
7	С	1	Total 98	C 56	N 7	O 35	0



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: Spike glycoprotein













• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

	100%		
Chain E:	50%	50%	
NAG2			
• Molecule 9	2 acatamida 2 daarre hata	D alucentranego (1	1) 2 a cotamida

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

	50%	
Chain X:	10	0%
•		

NAG1 NAG2

> IAG1 IAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

100%



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

	1	.00%	
Chain Z:	50%		50%
* *			
NAG2 NAG2			

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

	50%	
Chain d:	50%	50%
•		
NAG1 NAG2		

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain f:	50%	50%	
NAG1 NAG2			

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:	50%	0%
NAG1 NAG2		

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

		100%		
Chain N:	50%		50%	

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

		67%	
Chain k:	33%	67%	
• •			
AG1 AG2 UC3			
		WORLDWIDE	

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

	33%		
Chain p:		100%	
NAG NAG BMAG			

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-ac etamido-2-deoxy-beta-D-glucopyranose

	67%	_
Chain V:	100%	
••		
461 462 483		

 $\bullet \ Molecule \ 5: \ alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$

	100%				
Chain h:	50%	50%			
NAG1					

 $\bullet \ Molecule \ 6: \ alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose$

	75%
Chain Q:	100%

AG1 AG2 MA3 AN4	
N 19 W	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM $(4k \ge 4k)$	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00738	Depositor
Map size (Å)	354.24, 354.24, 354.24	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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).

Mal	Chain	Bo	nd lengths	Bond angles		
NIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.55	2/7900~(0.0%)	0.63	1/10764~(0.0%)	
1	В	0.54	0/7839	0.62	0/10679	
1	С	0.57	2/8069~(0.0%)	0.62	1/11005~(0.0%)	
All	All	0.55	4/23808~(0.0%)	0.62	2/32448~(0.0%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	330	PRO	N-CA	13.68	1.70	1.47
1	С	330	PRO	N-CA	13.67	1.70	1.47
1	А	329	PHE	C-N	6.05	1.45	1.34
1	С	329	PHE	C-N	6.05	1.45	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	330	PRO	CA-N-CD	-9.52	98.17	111.50
1	С	330	PRO	CA-N-CD	-8.38	99.76	111.50

There are no chirality outliers.

There are no planarity outliers.

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	Perce	entiles
1	А	995/1127~(88%)	780 (78%)	205 (21%)	10 (1%)	15	54
1	В	988/1127~(88%)	770 (78%)	206 (21%)	12 (1%)	13	50
1	С	1023/1127~(91%)	780 (76%)	231 (23%)	12 (1%)	13	50
All	All	3006/3381~(89%)	2330 (78%)	642 (21%)	34 (1%)	18	52

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	329	PHE
1	В	538	CYS
1	С	145	TYR
1	С	330	PRO
1	С	498	GLN
1	С	518	LEU
1	А	70	VAL
1	А	150	LYS
1	В	88	ASP
1	В	622	VAL
1	С	250	THR
1	С	252	GLY
1	С	454	ARG
1	А	617	CYS
1	В	78	ARG
1	В	85	PRO
1	А	69	HIS
1	А	151	SER
1	В	153	MET
1	В	295	PRO
1	А	186	PHE
1	A	1030	SER
1	В	74	ASN
1	В	605	SER



Mol	Chain	Res	Type
1	В	783	ALA
1	В	823	PHE
1	С	749	CYS
1	С	812	PRO
1	С	247	SER
1	А	798	GLY
1	А	1079	PRO
1	С	798	GLY
1	В	491	PRO
1	С	272	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	838/976~(86%)	812~(97%)	26~(3%)	40 62
1	В	827/976~(85%)	809~(98%)	18 (2%)	52 71
1	С	850/976~(87%)	827 (97%)	23 (3%)	44 66
All	All	2515/2928~(86%)	2448 (97%)	67 (3%)	48 66

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	52	GLN
1	А	70	VAL
1	А	150	LYS
1	А	153	MET
1	А	186	PHE
1	А	245	HIS
1	А	248	TYR
1	А	278	LYS
1	А	302	THR
1	А	317	ASN
1	А	331	ASN
1	А	391	CYS



Mol	Chain	Res	Type
1	А	525	CYS
1	А	538	CYS
1	А	565	PHE
1	А	568	ASP
1	А	649	CYS
1	А	662	CYS
1	А	732	THR
1	А	770	ILE
1	А	854	LYS
1	А	873	TYR
1	А	886	TRP
1	А	1047	TYR
1	А	1058	HIS
1	A	1118	ASP
1	В	32	PHE
1	В	58	PHE
1	В	138	ASP
1	В	144	TYR
1	В	147	LYS
1	В	315	THR
1	В	336	CYS
1	В	342	PHE
1	В	421	TYR
1	В	497	PHE
1	В	508	TYR
1	В	763	LEU
1	В	811	LYS
1	В	813	SER
1	В	814	LYS
1	В	854	LYS
1	В	869	MET
1	В	1027	THR
1	С	44	ARG
1	С	122	ASN
1	С	145	TYR
1	С	253	ASP
1	С	331	ASN
1	С	334	ASN
1	С	355	ARG
1	С	403	ARG
1	C	455	LEU
1	С	457	ARG



Mol	Chain	Res	Type
1	С	459	SER
1	С	505	TYR
1	С	514	SER
1	С	515	PHE
1	С	544	ASN
1	С	547	THR
1	С	567	ARG
1	С	590	CYS
1	С	699	LEU
1	C	763	LEU
1	С	770	ILE
1	С	1042	PHE
1	С	1101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	81	ASN
1	А	87	ASN
1	А	99	ASN
1	А	125	ASN
1	А	134	GLN
1	А	146	HIS
1	А	148	ASN
1	А	207	HIS
1	А	613	GLN
1	А	641	ASN
1	А	655	HIS
1	А	658	ASN
1	А	751	ASN
1	А	777	ASN
1	А	787	GLN
1	А	901	GLN
1	А	920	GLN
1	А	928	ASN
1	А	935	GLN
1	А	949	GLN
1	А	953	ASN
1	А	969	ASN
1	А	1010	GLN
1	А	1048	HIS
1	А	1054	GLN



Mol	Chain	Res	Type
1	A	1088	HIS
1	А	1108	ASN
1	В	49	HIS
1	В	87	ASN
1	В	121	ASN
1	В	185	ASN
1	В	388	ASN
1	В	506	GLN
1	В	542	ASN
1	В	564	GLN
1	В	607	GLN
1	В	655	HIS
1	В	764	ASN
1	В	784	GLN
1	В	953	ASN
1	В	954	GLN
1	В	992	GLN
1	В	1048	HIS
1	В	1071	GLN
1	В	1083	HIS
1	В	1101	HIS
1	В	1113	GLN
1	С	49	HIS
1	С	66	HIS
1	С	146	HIS
1	С	188	ASN
1	С	207	HIS
1	C	245	HIS
1	C	280	ASN
1	C	460	ASN
1	C	506	GLN
1	С	644	GLN
1	C	804	GLN
1	C	965	GLN
1	C	978	ASN
1	C	992	GLN
1	С	1048	HIS
1	С	1108	ASN
1	С	1135	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)

33 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).

Mal	Turne	Chain	Res	Tink	Bo	ond leng	ths	В	ond ang	les
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	Е	1	2,1	14,14,15	0.42	0	17,19,21	0.49	0
2	NAG	Е	2	2	14,14,15	0.47	0	17,19,21	1.24	1 (5%)
2	NAG	Н	1	2,1	14,14,15	0.49	0	17,19,21	0.53	0
2	NAG	Н	2	2	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	Ν	1	2,1	14,14,15	0.62	0	17,19,21	1.10	1 (5%)
2	NAG	N	2	2	14,14,15	0.40	0	17,19,21	0.36	0
6	NAG	Q	1	6,1	14,14,15	1.76	1 (7%)	17,19,21	1.54	3 (17%)
6	NAG	Q	2	6	14,14,15	0.29	0	17,19,21	0.78	1 (5%)
6	BMA	Q	3	6	11,11,12	0.85	1 (9%)	$15,\!15,\!17$	0.96	1 (6%)
6	MAN	Q	4	6	11,11,12	0.96	1 (9%)	$15,\!15,\!17$	1.66	2 (13%)
4	NAG	V	1	4,1	14,14,15	0.26	0	17,19,21	0.67	0
4	NAG	V	2	4	14,14,15	0.27	0	17,19,21	0.68	0
4	BMA	V	3	4	11,11,12	0.24	0	$15,\!15,\!17$	0.86	0
2	NAG	W	1	2,1	14,14,15	0.75	1(7%)	17,19,21	0.73	0
2	NAG	W	2	2	14,14,15	0.85	2 (14%)	17,19,21	0.73	0
2	NAG	Х	1	2,1	14,14,15	0.29	0	17,19,21	0.65	0
2	NAG	Х	2	2	14,14,15	0.31	0	17,19,21	0.63	0
2	NAG	Z	1	2,1	14,14,15	0.61	1 (7%)	17,19,21	0.46	0
2	NAG	Z	2	2	14,14,15	0.29	0	17,19,21	0.57	0
2	NAG	d	1	2,1	14,14,15	0.52	0	17,19,21	0.61	0



Mal	Turne	Type Chain Bes Link		T in le	Bo	ond leng	ths	Bond angles		
IVIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	d	2	2	14,14,15	0.16	0	17,19,21	0.85	1 (5%)
2	NAG	f	1	2,1	14,14,15	0.71	1 (7%)	17,19,21	0.48	0
2	NAG	f	2	2	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	h	1	1,5	14,14,15	0.36	0	17,19,21	0.74	0
5	NAG	h	2	5	14,14,15	0.25	0	17,19,21	0.82	1 (5%)
5	BMA	h	3	5	11,11,12	0.74	0	15,15,17	0.85	0
5	MAN	h	4	5	11,11,12	0.82	1 (9%)	15,15,17	1.39	3 (20%)
3	NAG	k	1	3,1	14,14,15	0.32	0	17,19,21	0.54	0
3	NAG	k	2	3	14,14,15	0.42	0	17,19,21	0.99	1 (5%)
3	FUC	k	3	3	10,10,11	0.88	0	14,14,16	1.80	2 (14%)
4	NAG	р	1	4,1	14,14,15	0.37	0	17,19,21	0.78	0
4	NAG	р	2	4	14, 14, 15	0.33	0	17,19,21	0.66	0
4	BMA	р	3	4	11,11,12	0.27	0	15,15,17	0.70	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	Е	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Е	2	2	-	3/6/23/26	0/1/1/1
2	NAG	Н	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Н	2	2	-	4/6/23/26	0/1/1/1
2	NAG	Ν	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	Ν	2	2	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	3/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	0/2/19/22	0/1/1/1
4	NAG	V	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	BMA	V	3	4	-	0/2/19/22	0/1/1/1
2	NAG	W	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	NAG	Х	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	Х	2	2	-	5/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	1/6/23/26	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Z	2	2	-	3/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	0/1/1/1
2	NAG	f	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	f	2	2	-	4/6/23/26	0/1/1/1
5	NAG	h	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	h	2	5	-	1/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	MAN	h	4	5	-	1/2/19/22	0/1/1/1
3	NAG	k	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	k	2	3	-	3/6/23/26	0/1/1/1
3	FUC	k	3	3	-	-	0/1/1/1
4	NAG	р	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	р	2	4	-	5/6/23/26	0/1/1/1
4	BMA	р	3	4	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
6	Q	1	NAG	O5-C1	-6.50	1.33	1.43
2	W	1	NAG	O5-C1	-2.75	1.39	1.43
5	h	4	MAN	C1-C2	2.31	1.57	1.52
2	Ζ	1	NAG	O5-C1	-2.19	1.40	1.43
2	W	2	NAG	C1-C2	2.15	1.55	1.52
6	Q	3	BMA	O3-C3	-2.09	1.38	1.43
2	f	1	NAG	O5-C1	-2.09	1.40	1.43
2	W	2	NAG	O5-C1	-2.08	1.40	1.43
6	Q	4	MAN	C1-C2	-2.05	1.47	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	Q	4	MAN	C1-O5-C5	4.68	118.53	112.19
6	Q	1	NAG	C2-N2-C7	4.30	129.03	122.90
2	Е	2	NAG	C2-N2-C7	4.19	128.87	122.90
3	k	3	FUC	C1-O5-C5	4.01	121.87	112.78
3	k	3	FUC	O5-C5-C4	3.88	116.48	109.52
3	k	2	NAG	C1-O5-C5	3.11	116.41	112.19
2	Ν	1	NAG	C1-O5-C5	3.04	116.31	112.19
6	Q	4	MAN	C1-C2-C3	-2.78	106.25	109.67



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	d	2	NAG	C1-O5-C5	2.76	115.93	112.19
5	h	4	MAN	C1-O5-C5	2.76	115.93	112.19
5	h	4	MAN	O2-C2-C3	-2.65	104.83	110.14
6	Q	1	NAG	C1-O5-C5	-2.43	108.90	112.19
6	Q	2	NAG	C1-O5-C5	2.34	115.36	112.19
5	h	2	NAG	C1-O5-C5	2.32	115.34	112.19
5	h	4	MAN	C1-C2-C3	2.24	112.42	109.67
6	Q	3	BMA	C3-C4-C5	-2.19	106.33	110.24
6	Q	1	NAG	O4-C4-C5	-2.18	103.88	109.30

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Х	1	NAG	C3-C2-N2-C7
2	Х	1	NAG	O7-C7-N2-C2
4	р	2	NAG	C3-C2-N2-C7
4	V	1	NAG	C3-C2-N2-C7
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
2	Х	1	NAG	C8-C7-N2-C2
4	р	1	NAG	C8-C7-N2-C2
4	р	1	NAG	O7-C7-N2-C2
2	Е	1	NAG	O5-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	W	2	NAG	C1-C2-N2-C7
4	р	3	BMA	O5-C5-C6-O6
2	Н	1	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
2	Ζ	2	NAG	C4-C5-C6-O6
2	Н	2	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	f	2	NAG	O5-C5-C6-O6
6	Q	1	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
2	Н	1	NAG	C4-C5-C6-O6
2	Е	1	NAG	C4-C5-C6-O6
4	р	3	BMA	C4-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	Н	2	NAG	O5-C5-C6-O6
2	d	1	NAG	C1-C2-N2-C7



Mol	Chain	Res	Type	Atoms
4	р	1	NAG	C1-C2-N2-C7
3	k	1	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	Е	2	NAG	C8-C7-N2-C2
2	Е	2	NAG	O7-C7-N2-C2
2	Х	2	NAG	C8-C7-N2-C2
2	f	2	NAG	C8-C7-N2-C2
2	f	2	NAG	O7-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
2	N	2	NAG	O5-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Q	1	NAG	C4-C5-C6-O6
2	f	2	NAG	C4-C5-C6-O6
3	k	1	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	Х	2	NAG	O7-C7-N2-C2
2	d	2	NAG	O5-C5-C6-O6
2	Ν	2	NAG	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
2	Х	2	NAG	C1-C2-N2-C7
5	h	4	MAN	O5-C5-C6-O6
3	k	1	NAG	C1-C2-N2-C7
5	h	2	NAG	O5-C5-C6-O6
2	Х	2	NAG	O5-C5-C6-O6
2	Х	2	NAG	C3-C2-N2-C7
3	k	2	NAG	C4-C5-C6-O6
2	Х	1	NAG	O5-C5-C6-O6
2	Н	2	NAG	C1-C2-N2-C7
4	р	2	NAG	C4-C5-C6-O6
4	р	2	NAG	C8-C7-N2-C2
4	р	2	NAG	O5-C5-C6-O6
2	Z	1	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
2	W	1	NAG	C3-C2-N2-C7
2	W	2	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
3	k	2	NAG	C3-C2-N2-C7



Mol	Chain	Res	Type	Atoms
6	Q	1	NAG	C3-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
4	р	2	NAG	O7-C7-N2-C2
2	Е	2	NAG	C3-C2-N2-C7
2	Н	2	NAG	C3-C2-N2-C7
3	k	1	NAG	C3-C2-N2-C7

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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)

23 ligands are modelled in this entry.



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

Mal	Type	Chain	Dog	Link	Bo	ond leng	$_{\rm sths}$	Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	В	1202	1	14,14,15	0.39	0	17,19,21	0.61	0
7	NAG	А	1206	1	14,14,15	0.27	0	17,19,21	0.46	0
7	NAG	В	1203	1	14,14,15	0.59	1 (7%)	17,19,21	0.54	0
7	NAG	С	1201	1	14,14,15	0.22	0	17,19,21	0.55	0
7	NAG	В	1201	1	14,14,15	0.27	0	17,19,21	0.62	0
7	NAG	С	1205	1	14,14,15	0.30	0	17,19,21	0.58	0
7	NAG	В	1205	1	14,14,15	1.65	1 (7%)	17,19,21	0.97	1 (5%)
7	NAG	С	1206	1	14,14,15	0.49	0	17,19,21	1.17	2 (11%)
7	NAG	В	1204	1	14,14,15	0.47	0	17,19,21	1.23	1 (5%)
7	NAG	А	1207	1	14,14,15	0.92	1 (7%)	17,19,21	1.41	2 (11%)
7	NAG	В	1208	1	14,14,15	0.80	1 (7%)	17,19,21	0.52	0
7	NAG	В	1206	1	14,14,15	0.21	0	17,19,21	0.70	1 (5%)
7	NAG	С	1204	-	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
7	NAG	В	1209	1	14,14,15	0.27	0	17,19,21	0.69	0
7	NAG	С	1207	1	14,14,15	0.26	0	17,19,21	0.72	0
7	NAG	А	1203	1	14,14,15	0.29	0	17,19,21	0.61	0
7	NAG	С	1203	1	14,14,15	0.38	0	17,19,21	0.45	0
7	NAG	А	1202	1	$14,\!14,\!15$	0.20	0	17,19,21	0.55	0
7	NAG	А	1201	1	$14,\!14,\!15$	0.59	0	17,19,21	0.80	0
7	NAG	В	1207	1	$14,\!14,\!15$	0.29	0	17,19,21	0.40	0
7	NAG	C	1202	1	14,14,15	0.69	1 (7%)	17,19,21	1.25	2 (11%)
7	NAG	А	1205	1	$14,\!14,\!15$	0.40	0	17,19,21	1.41	2 (11%)
7	NAG	A	1204	1	$1\overline{4,}14,15$	0.23	0	17,19,21	0.64	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
7	NAG	В	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	А	1206	1	-	1/6/23/26	0/1/1/1

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	В	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	С	1201	1	-	2/6/23/26	0/1/1/1
7	NAG	В	1201	1	-	3/6/23/26	0/1/1/1
7	NAG	С	1205	1	-	4/6/23/26	0/1/1/1
7	NAG	В	1205	1	-	4/6/23/26	0/1/1/1
7	NAG	С	1206	1	-	3/6/23/26	0/1/1/1
7	NAG	В	1204	1	-	5/6/23/26	0/1/1/1
7	NAG	А	1207	1	-	4/6/23/26	0/1/1/1
7	NAG	В	1208	1	-	2/6/23/26	0/1/1/1
7	NAG	В	1206	1	-	2/6/23/26	0/1/1/1
7	NAG	С	1204	-	-	1/6/23/26	0/1/1/1
7	NAG	В	1209	1	-	1/6/23/26	0/1/1/1
7	NAG	С	1207	1	-	0/6/23/26	0/1/1/1
7	NAG	А	1203	1	-	0/6/23/26	0/1/1/1
7	NAG	С	1203	1	-	4/6/23/26	0/1/1/1
7	NAG	А	1202	1	-	2/6/23/26	0/1/1/1
7	NAG	А	1201	1	-	3/6/23/26	0/1/1/1
7	NAG	В	1207	1	-	2/6/23/26	0/1/1/1
7	NAG	С	1202	1	-	5/6/23/26	0/1/1/1
7	NAG	А	1205	1	-	3/6/23/26	0/1/1/1
7	NAG	А	1204	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
7	В	1205	NAG	O5-C1	-5.83	1.34	1.43
7	А	1207	NAG	C1-C2	3.03	1.56	1.52
7	В	1208	NAG	O5-C1	-2.58	1.39	1.43
7	С	1202	NAG	O5-C1	-2.36	1.40	1.43
7	В	1203	NAG	C1-C2	2.01	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	А	1205	NAG	C2-N2-C7	4.43	129.22	122.90
7	В	1204	NAG	C2-N2-C7	4.26	128.97	122.90
7	С	1202	NAG	C2-N2-C7	4.11	128.75	122.90
7	А	1207	NAG	C2-N2-C7	3.85	128.38	122.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	С	1206	NAG	C2-N2-C7	3.51	127.90	122.90
7	А	1207	NAG	C1-O5-C5	3.31	116.67	112.19
7	В	1205	NAG	C3-C4-C5	2.84	115.30	110.24
7	А	1205	NAG	C1-C2-N2	2.69	115.08	110.49
7	С	1204	NAG	C1-O5-C5	2.35	115.38	112.19
7	В	1206	NAG	C1-O5-C5	2.27	115.27	112.19
7	С	1206	NAG	C1-C2-N2	2.09	114.05	110.49
7	С	1202	NAG	C1-C2-N2	2.06	114.01	110.49

There are no chirality outliers.

All	(59)	torsion	outliers	are	listed	below:	

Mol	Chain	\mathbf{Res}	Type	Atoms
7	В	1209	NAG	C3-C2-N2-C7
7	В	1208	NAG	O5-C5-C6-O6
7	А	1202	NAG	C4-C5-C6-O6
7	В	1204	NAG	O5-C5-C6-O6
7	В	1206	NAG	C4-C5-C6-O6
7	В	1206	NAG	O5-C5-C6-O6
7	В	1202	NAG	O5-C5-C6-O6
7	В	1208	NAG	C4-C5-C6-O6
7	В	1203	NAG	O5-C5-C6-O6
7	А	1202	NAG	O5-C5-C6-O6
7	С	1203	NAG	O5-C5-C6-O6
7	А	1201	NAG	C1-C2-N2-C7
7	С	1203	NAG	C4-C5-C6-O6
7	А	1205	NAG	C8-C7-N2-C2
7	А	1205	NAG	O7-C7-N2-C2
7	А	1207	NAG	C8-C7-N2-C2
7	А	1207	NAG	O7-C7-N2-C2
7	В	1204	NAG	C8-C7-N2-C2
7	В	1204	NAG	O7-C7-N2-C2
7	С	1202	NAG	C8-C7-N2-C2
7	С	1202	NAG	O7-C7-N2-C2
7	С	1203	NAG	C8-C7-N2-C2
7	С	1203	NAG	O7-C7-N2-C2
7	С	1205	NAG	C8-C7-N2-C2
7	С	1205	NAG	O7-C7-N2-C2
7	С	1206	NAG	C8-C7-N2-C2
7	С	1206	NAG	O7-C7-N2-C2
7	В	1207	NAG	O5-C5-C6-O6
7	В	1205	NAG	O5-C5-C6-O6



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Mol	Chain	Res	Type	Atoms	
7	В	1203	NAG	C4-C5-C6-O6	
7	В	1205	NAG	C4-C5-C6-O6	
7	В	1204	NAG	C4-C5-C6-O6	
7	В	1203	NAG	C1-C2-N2-C7	
7	А	1204	NAG	O5-C5-C6-O6	
7	А	1201	NAG	O5-C5-C6-O6	
7	7 B		NAG	C1-C2-N2-C7	
7	С	1205	NAG	O5-C5-C6-O6	
7	В	1201	NAG	O5-C5-C6-O6	
7	С	1202	NAG	C4-C5-C6-O6	
7	С	1201	NAG	C4-C5-C6-O6	
7	С	1202	NAG	O5-C5-C6-O6	
7	А	1207	NAG	C4-C5-C6-O6	
7	А	1204	NAG	C4-C5-C6-O6	
7	А	1206	NAG	C1-C2-N2-C7	
7	А	1201	NAG	C3-C2-N2-C7	
7	А	1205	NAG	C3-C2-N2-C7	
7	В	1201	NAG	C3-C2-N2-C7	
7	В	1205	NAG	C3-C2-N2-C7	
7	С	1202	NAG	C3-C2-N2-C7	
7	С	1204	NAG	C3-C2-N2-C7	
7	С	1205	NAG	C3-C2-N2-C7	
7	С	1201	NAG	O5-C5-C6-O6	
7	В	1202	NAG	C4-C5-C6-O6	
7	В	1207	NAG	C4-C5-C6-O6	
7	В	1201	NAG	C4-C5-C6-O6	
7	A	1207	NAG	C3-C2-N2-C7	
7	В	1203	NAG	C3-C2-N2-C7	
7	В	1204	NAG	C3-C2-N2-C7	
7	С	1206	NAG	C3-C2-N2-C7	

Continued from previous page...

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30419. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



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: 207

Y Index: 213

Z Index: 224

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00738. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 92 nm^3 ; this corresponds to an approximate mass of 84 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 0.213 \AA^{-1}



8 Fourier-Shell correlation (i)

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



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30419 and PDB model 7CN9. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.00738 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00738).



9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00738) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.4247	0.3410	
A	0.3973	0.3420	
В	0.4409	0.3360	10
C	0.4447	0.3410	
E	0.1071	0.4070	
Н	0.3571	0.3700	
N	0.0714	0.4400	
Q	0.2200	0.3940	
V	0.2308	0.2700	
W	0.4643	0.4540	
X	0.2857	0.4050	
Z	0.0000	0.4640	0.0
d	0.3214	0.4190	<0.0
f	0.5357	0.4710	
h	0.0800	0.4670	
k	0.3947	0.4780	
р	0.4103	0.3900	

