

wwPDB EM Validation Summary Report (i)

Dec 2, 2024 – 02:24 PM JST

PDB ID	:	8YZI
EMDB ID	:	EMD-39694
Title	:	The structure of PDCoV RBD and dog APN complex
Authors	:	Sun, J.Q.; Niu, S.
Deposited on		
Resolution	:	3.05 Å(reported)

This is a wwPDB EM Validation Summary 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 (i)) were used in the production of this report:

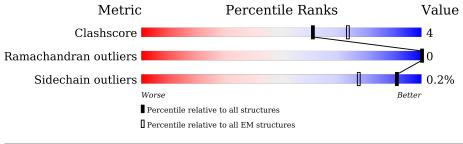
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.05 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	А	132	• 66%	21%	13%
1	С	132	• 69%	18%	13%
2	В	940	84%		12% •
2	D	940	87%		9% •
3	Е	2	50%	50%	
3	F	2	100%		
3	Н	2	100%		
3	Ι	2	100%		



Conti	Continued from previous page							
Mol	Chain	Length	Quality of	f chain				
3	J	2	50%	50%				
3	Κ	2	100%					
3	L	2	100%					
3	М	2	100%					
3	Ν	2	50%	50%				
4	G	2	100%					

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16699 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	С	115	Total	С	Ν	0	\mathbf{S}	0	0
1 I	U	110	898	560	149	178	11	0	0
1	Λ	115	Total	С	Ν	Ο	\mathbf{S}	0	0
	А	115	898	560	149	178	11		0

• Molecule 1 is a protein called Spike protein.

• Molecule 2 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	В	900	Total 7263	-		0 1373	S 23	0	0
2	D	900	Total 7263	-		0 1373	S 23	0	0

• Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	A	Aton	ns		AltConf	Trace
3	Е	2	Total	С	Ν	0	Ο	0
0	Ľ	2	28	16	2	10	0	0
3	F	2	Total	\mathbf{C}	Ν	0	0	0
0	Ľ	2	28	16	2	10	0	0
3	Н	2	Total	\mathbf{C}	Ν	Ο	0	0
0	11		28	16	2	10	0	0
3	Т	2	Total	\mathbf{C}	Ν	Ο	0	0
0	1		28	16	2	10	0	0
3	J	2	Total	С	Ν	Ο	0	0
0	5		28	16	2	10	0	0
3	Κ	2	Total	С	Ν	Ο	0	0
	17	2	28	16	2	10		0



Conti	nueu jron	i previous pa	<i>ge</i>		
Mol	Chain	Residues	Atoms	AltConf	Trace
3	L	2	Total C N O 28 16 2 10	0	0
3	М	2	Z0 I0 Z I0 Total C N O 28 16 2 10	0	0
3	Ν	2	Total C N O 28 16 2 10	0	0

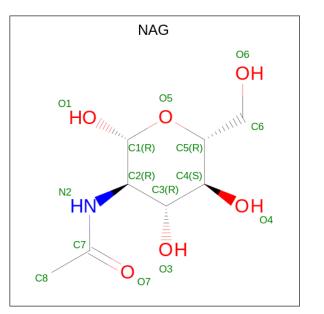
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• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
4	G	2	Total 25	C 14	N 1	O 10	0	0

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
Б	С	1	Total	С	Ν	0	0
0	U		14	8	1	5	0
5	Δ	1	Total	С	Ν	Ο	0
0	A	1	14	8	1	5	0



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Mol	Chain	Residues	Atoms	AltConf
5	В	1	Total C N O	0
			14 8 1 5	_
5	В	1	Total C N O	0
0	D	1	14 8 1 5	0
5	В	1	Total C N O	0
0	D	1	14 8 1 5	0
5	D	1	Total C N O	0
0	D	1	14 8 1 5	0
5	Л	1	Total C N O	0
0	D	1	14 8 1 5	0

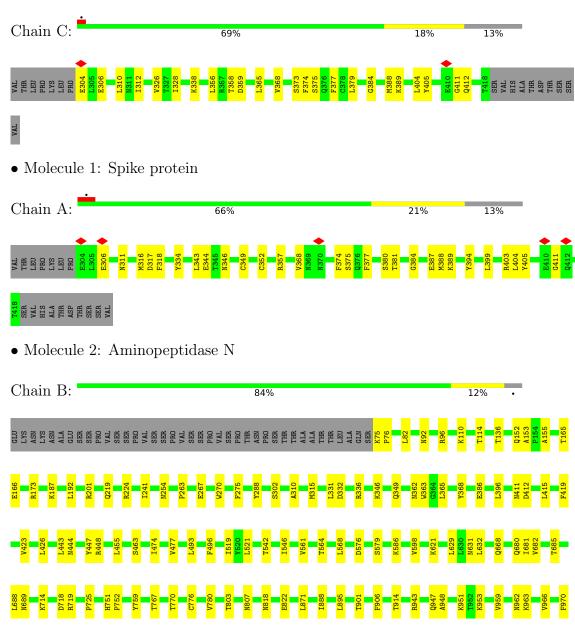
• Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
6	В	1	Total Zn 1 1	0
6	D	1	Total Zn 1 1	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 protein





• Molecule 2: Aminopeptidase N

(Ch	ai	n	D	: •				-											87	%	-													_	9%)	·				
GLU	LYS	ASN LYS	ASN	ALA	GLU	SER	VAL.	SER	SER	PRO VAL	SER	SER	VAL.	SER	SER	VAL	SER	PRO THR	ASN	PRO	SER THR	THR	ALA	THR	THR	LEU	GLN	SER V75		L82	H129	1138	Q139	P154	-	E174 P175	L176	V187	7011	L192	D195	L196
-	R201	D 222		K225	T238	F239	TO7 R		T283	Y284 L285	-	T300	V304		1308	R325		1330	Y342	P343	0349		N356	N362		L365	<mark>0378</mark>	NA03		A431	T470	0473	1474	V477		R491 M492	L493	S494	E499	D500		W524
-	N533	<mark>ຊ534</mark>	V598		L632 N633	V634	TGRE		1700	P725	-	R731	V734		F738	D750		T756	T767	A768	C769 T770		K775		P798	B801		C806	180 <mark>9</mark>	<mark>г816</mark>		V820	A839	T856		I862	Y 899	(1900	TOT	F906	1910	Q911
•	R915	D935		K951	N955	1956 7057		M969	F970	S974	GLN																															

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

α · π		
Chain E:	50%	50%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

100%





• Molecule 3:	eq:2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-a
opyranose	

50%

Chain J:

50%

NAG1 NAG2

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluc opyranose

Chain K:	100%
NAG1 NAG2	
• Molecule 3 opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-aceta
Chain L:	100%
NAG1 NAG2	
• Molecule 3 opyranose	2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-aceta
Chain M:	100%
NAG2 NAG2	
• Molecule 3 opyranose	$2\-acetamido-2\-deoxy\-beta-D\-glucopyranose\-(1-4)-2\-acetamido-2\-deoxy\-beta-D\-glucopyranose-(1-4)-2\-acetamido-2\-deoxy\-d$
Chain N:	50% 50%

Chain N:

NAG1 NAG2

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

Chain G:

100%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 $(6k \ge 4k)$	Depositor
Maximum map value	0.678	Depositor
Minimum map value	-0.208	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.141	Depositor
Map size (Å)	276.0, 276.0, 276.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.69, 0.69, 0.69	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: NAG, ZN, BMA

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
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/913	0.51	0/1238
1	С	0.24	0/913	0.51	0/1238
2	В	0.25	0/7457	0.48	0/10172
2	D	0.25	0/7457	0.47	0/10172
All	All	0.25	0/16740	0.48	0/22820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	А	898	0	859	17	0
1	С	898	0	859	15	0
2	В	7263	0	7059	63	0
2	D	7263	0	7060	47	0
3	Е	28	0	25	0	0
3	F	28	0	25	0	0
3	Н	28	0	25	0	0
3	Ι	28	0	25	0	0
3	J	28	0	25	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Κ	28	0	25	0	0
3	L	28	0	25	0	0
3	М	28	0	25	0	0
3	Ν	28	0	25	1	0
4	G	25	0	22	0	0
5	А	14	0	13	0	0
5	В	42	0	39	1	0
5	С	14	0	13	0	0
5	D	28	0	26	0	0
6	В	1	0	0	0	0
6	D	1	0	0	0	0
All	All	16699	0	16175	138	0

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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 4.

The worst 5 of 138 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:343:LEU:HD12	1:A:368:VAL:HG11	1.68	0.74
1:C:306:GLU:HB2	1:C:338:LYS:HD2	1.74	0.69
2:D:330:ILE:HD11	2:D:431:ALA:HB2	1.75	0.69
2:B:411:ASN:ND2	2:B:463:SER:O	2.23	0.69
1:C:359:ASP:HB2	1:C:389:LYS:HG3	1.74	0.68

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	А	113/132~(86%)	112 (99%)	1 (1%)	0	100 100		



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	С	113/132~(86%)	110~(97%)	3~(3%)	0	100	100
2	В	898/940~(96%)	866 (96%)	32~(4%)	0	100	100
2	D	898/940 (96%)	868~(97%)	30 (3%)	0	100	100
All	All	2022/2144~(94%)	1956 (97%)	66~(3%)	0	100	100

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There are no Ramachandran outliers to report.

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	103/119~(87%)	103 (100%)	0	100	100	
1	\mathbf{C}	103/119~(87%)	103 (100%)	0	100	100	
2	В	803/839~(96%)	800 (100%)	3 (0%)	89	93	
2	D	803/839~(96%)	802 (100%)	1 (0%)	92	96	
All	All	1812/1916~(95%)	1808 (100%)	4 (0%)	91	95	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	219	GLN
2	В	346	LYS
2	В	586	LYS
2	D	222	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type	
2	В	680	GLN	



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)

20 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	Bo	ond leng	ths	В	ond ang	les
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	Е	1	2,3	14,14,15	1.15	1 (7%)	17,19,21	1.00	1 (5%)
3	NAG	Е	2	3	14,14,15	0.37	0	17,19,21	0.34	0
3	NAG	F	1	2,3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	F	2	3	$14,\!14,\!15$	0.23	0	17,19,21	0.52	0
4	NAG	G	1	2,4	$14,\!14,\!15$	0.23	0	17,19,21	0.39	0
4	BMA	G	2	4	$11,\!11,\!12$	0.51	0	$15,\!15,\!17$	0.75	0
3	NAG	Н	1	2,3	$14,\!14,\!15$	0.44	0	17,19,21	0.60	0
3	NAG	Н	2	3	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	Ι	1	2,3	14,14,15	0.22	0	17,19,21	0.51	0
3	NAG	Ι	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	J	1	2,3	14,14,15	0.78	1 (7%)	17,19,21	0.78	1 (5%)
3	NAG	J	2	3	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	Κ	1	2,3	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	K	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	L	1	2,3	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	L	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	М	1	2,3	14,14,15	0.38	0	17,19,21	0.41	0
3	NAG	М	2	3	14,14,15	0.45	0	17,19,21	0.77	0
3	NAG	N	1	2,3	14,14,15	0.39	0	17,19,21	0.55	0
3	NAG	Ν	2	3	14,14,15	0.25	0	17,19,21	0.50	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	Е	1	2,3	-	3/6/23/26	0/1/1/1
3	NAG	Е	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
4	NAG	G	1	2,4	-	2/6/23/26	0/1/1/1
4	BMA	G	2	4	-	0/2/19/22	0/1/1/1
3	NAG	Н	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	Н	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Ι	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	Ι	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	2,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	Κ	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	М	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	М	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Ν	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	Ν	2	3	_	2/6/23/26	0/1/1/1

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.

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Е	1	NAG	O5-C1	-4.12	1.37	1.43
3	J	1	NAG	O5-C1	-2.80	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Е	1	NAG	C3-C4-C5	2.27	114.29	110.24
3	J	1	NAG	C3-C4-C5	2.12	114.02	110.24

There are no chirality outliers.

5 of 28 torsion outliers are listed below:



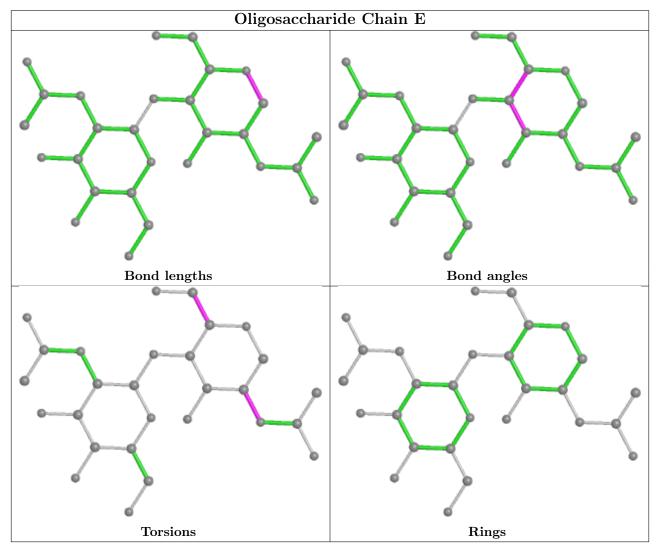
Mol	Chain	Res	Type	Atoms
3	Ι	1	NAG	C4-C5-C6-O6
3	М	2	NAG	O5-C5-C6-O6
3	Н	1	NAG	C4-C5-C6-O6
3	Н	1	NAG	O5-C5-C6-O6
3	Ι	1	NAG	O5-C5-C6-O6

There are no ring outliers.

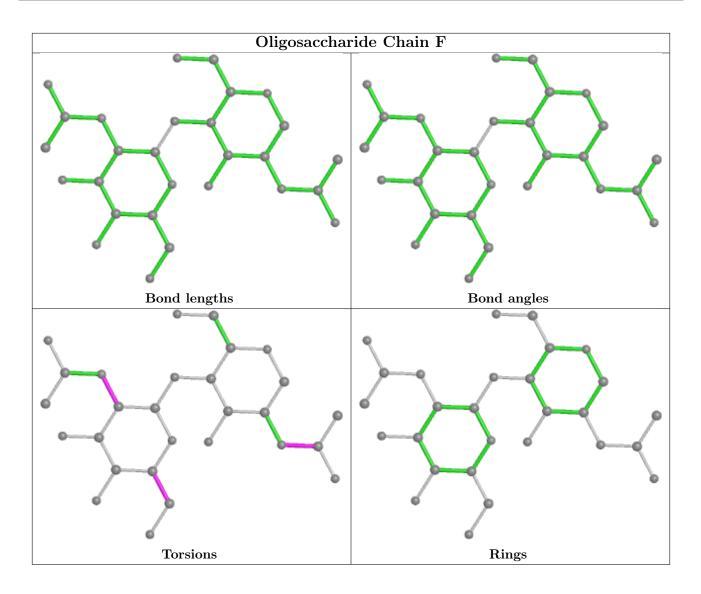
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ν	1	NAG	1	0

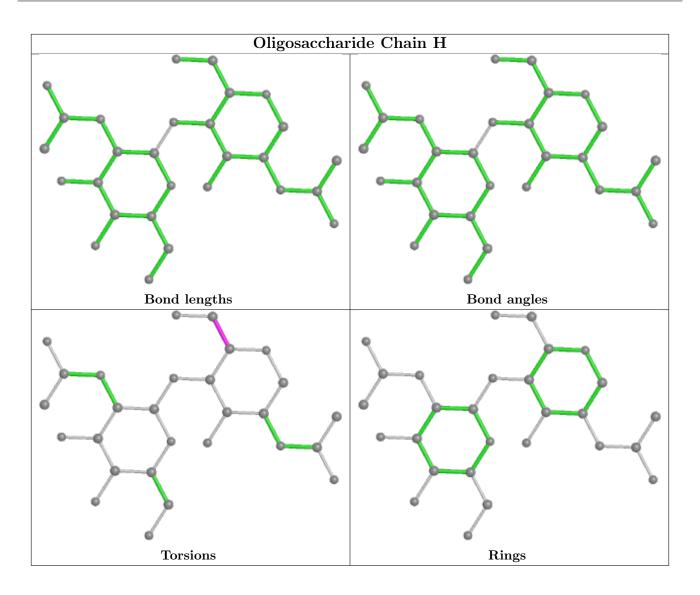
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



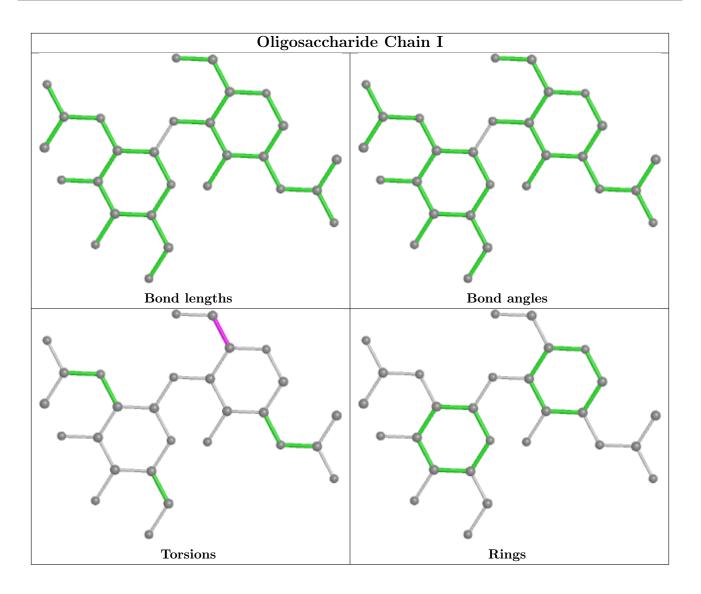




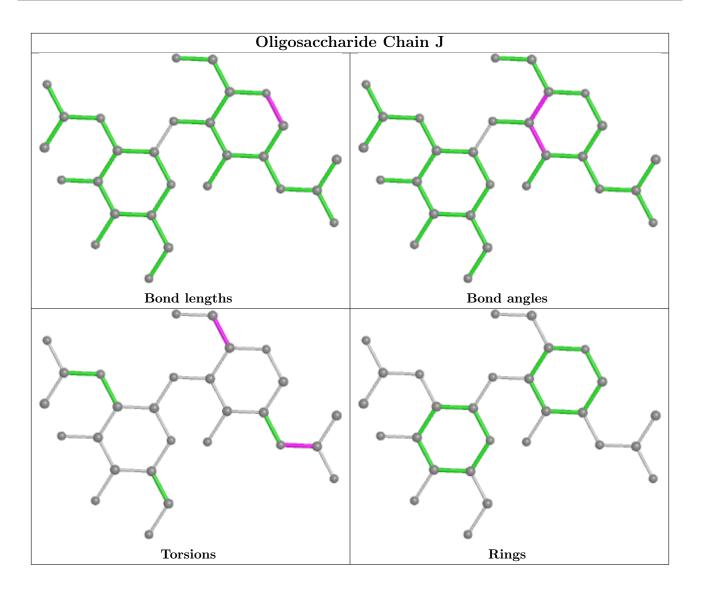




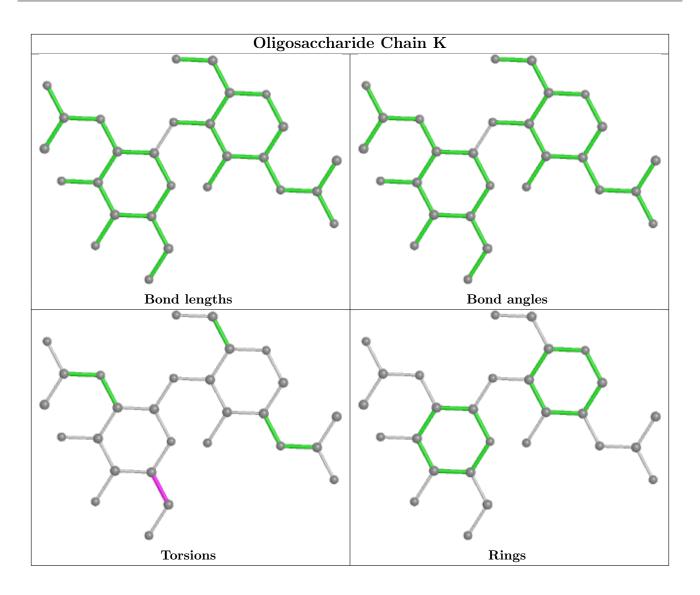




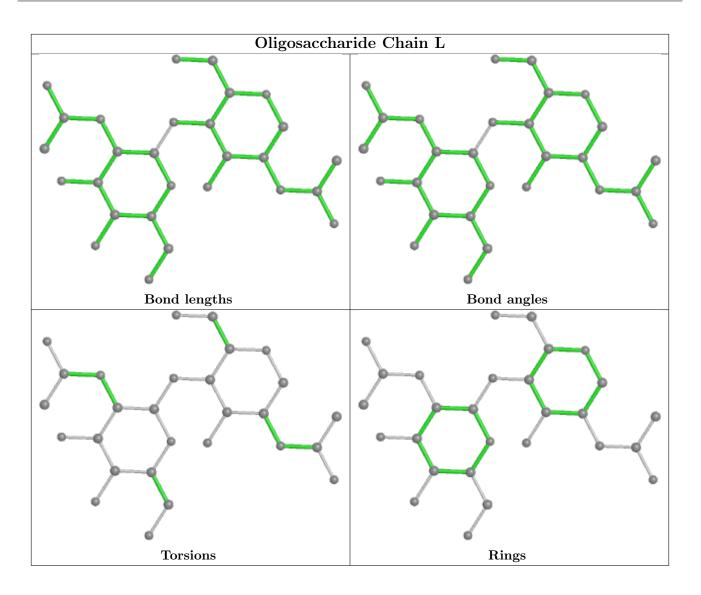




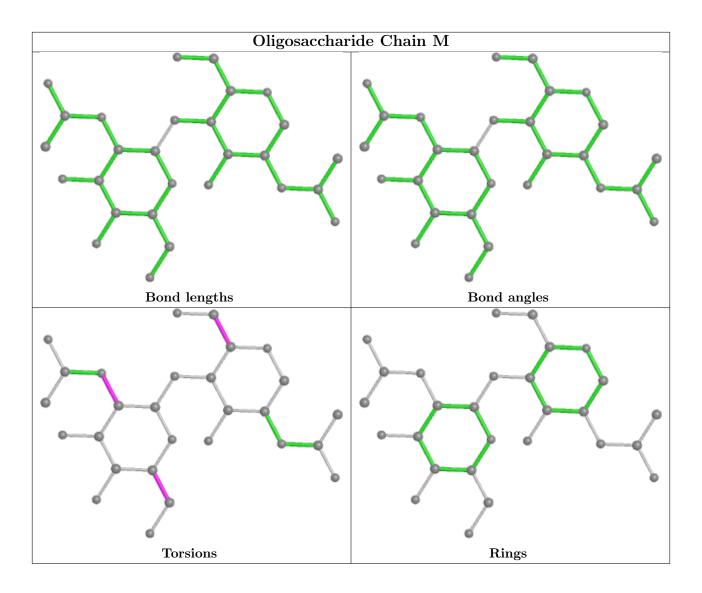




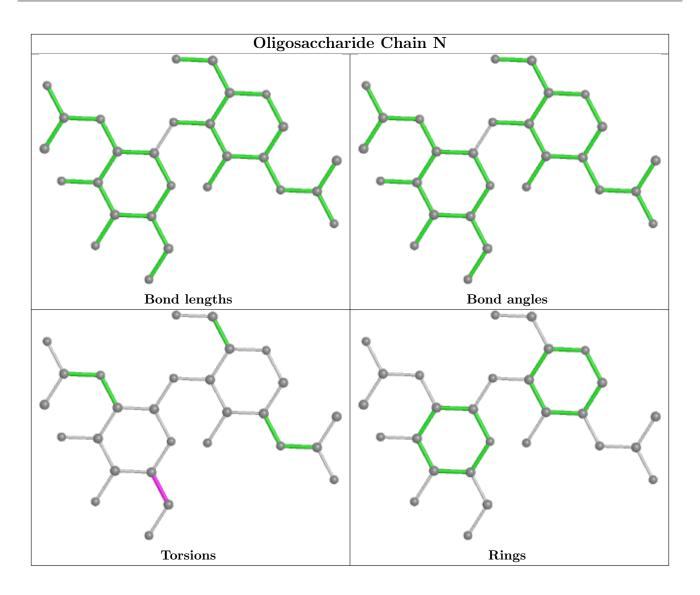




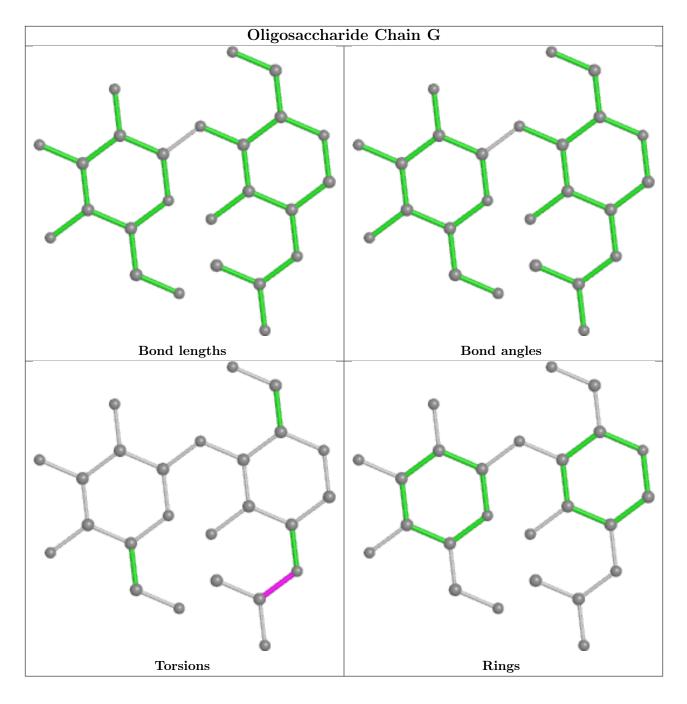












5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	Turne	Chain	Res	Link	Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	NAG	В	1003	2	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	С	501	1	$14,\!14,\!15$	0.19	0	17,19,21	0.40	0
5	NAG	D	1002	2	14,14,15	0.27	0	17,19,21	0.54	0
5	NAG	А	501	1	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	D	1001	2	$14,\!14,\!15$	0.22	0	17,19,21	0.43	0
5	NAG	В	1002	2	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	В	1001	2	$14,\!14,\!15$	0.22	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
5	NAG	В	1003	2	-	2/6/23/26	0/1/1/1
5	NAG	С	501	1	-	0/6/23/26	0/1/1/1
5	NAG	D	1002	2	-	2/6/23/26	0/1/1/1
5	NAG	А	501	1	-	2/6/23/26	0/1/1/1
5	NAG	D	1001	2	-	4/6/23/26	0/1/1/1
5	NAG	В	1002	2	-	3/6/23/26	0/1/1/1
5	NAG	В	1001	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1001	NAG	C4-C5-C6-O6
5	D	1001	NAG	O5-C5-C6-O6
5	В	1001	NAG	C4-C5-C6-O6
5	D	1002	NAG	C4-C5-C6-O6
5	А	501	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
5	В	1002	NAG	1	0



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.



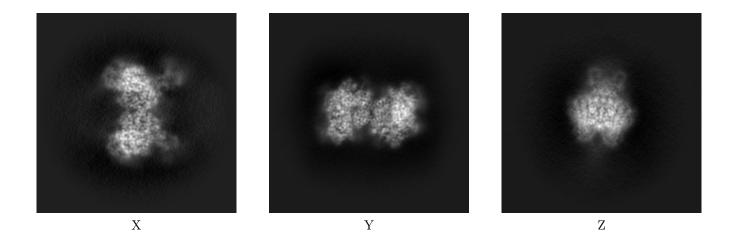
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39694. These allow visual inspection of the internal detail of the map and identification of artifacts.

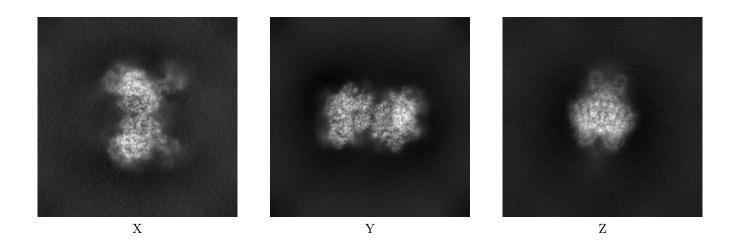
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

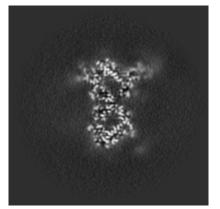


The images above show the map projected in three orthogonal directions.

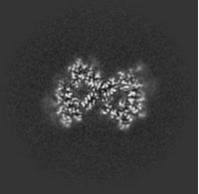


6.2Central slices (i)

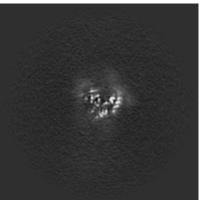
Primary map 6.2.1



X Index: 200

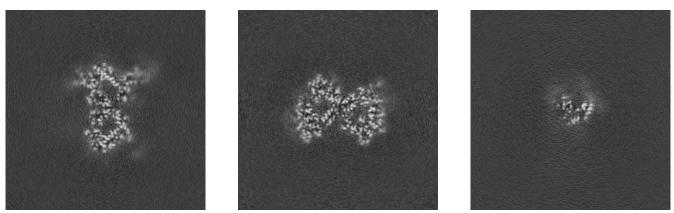


Y Index: 200



Z Index: 200

6.2.2Raw map



X Index: 200

Y Index: 200

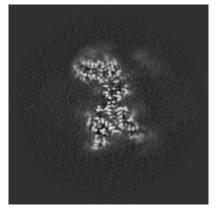


The images above show central slices of the map in three orthogonal directions.

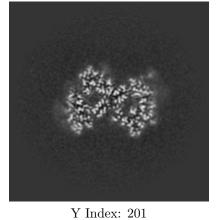


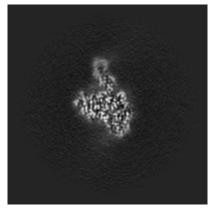
6.3 Largest variance slices (i)

6.3.1 Primary map



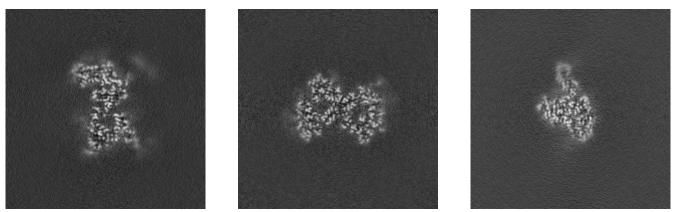
X Index: 220





Z Index: 260

6.3.2 Raw map



X Index: 215

Y Index: 201

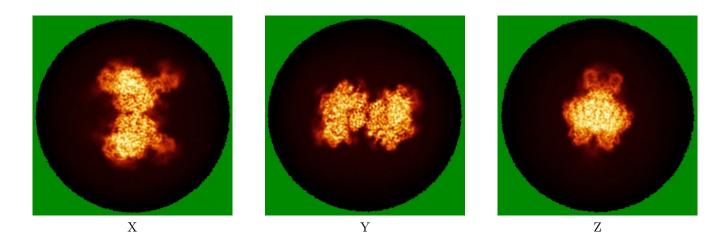


The images above show the largest variance slices of the map in three orthogonal directions.

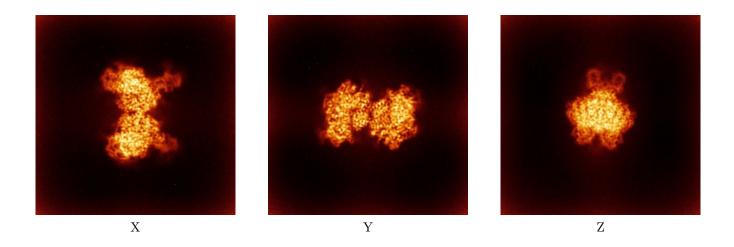


6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map

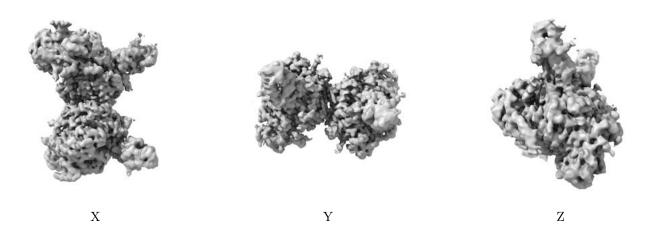


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



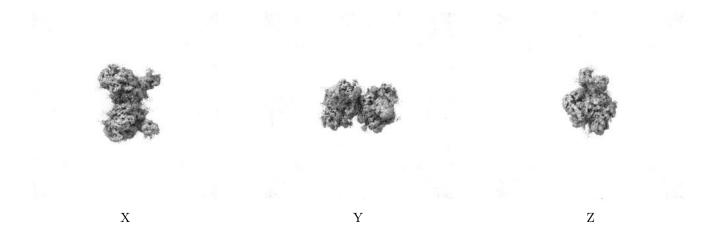
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.141. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

6.6 Mask visualisation (i)

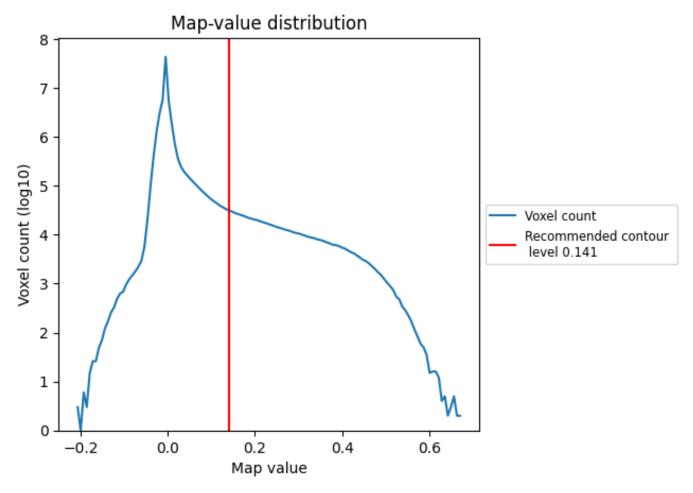
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

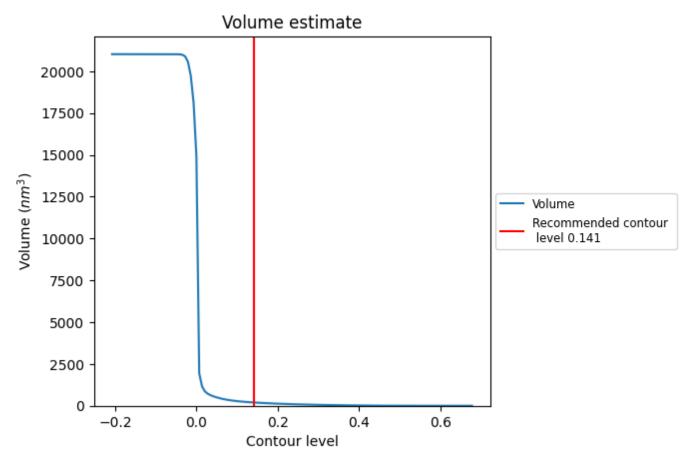
7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)

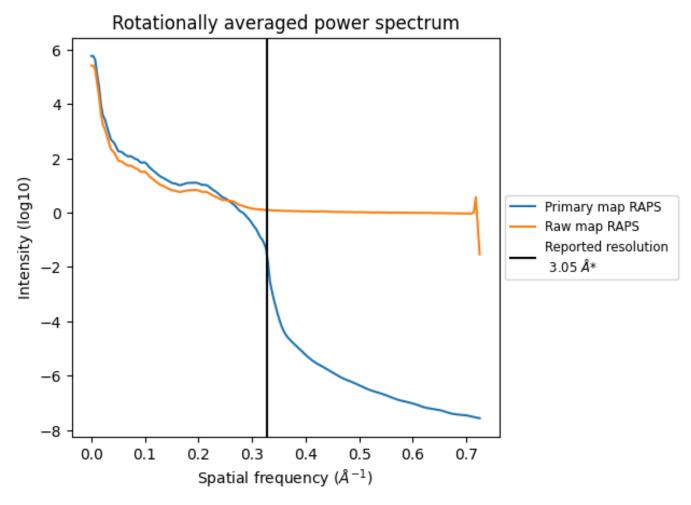


The volume at the recommended contour level is 197 $\rm nm^3;$ this corresponds to an approximate mass of 178 kDa.

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)



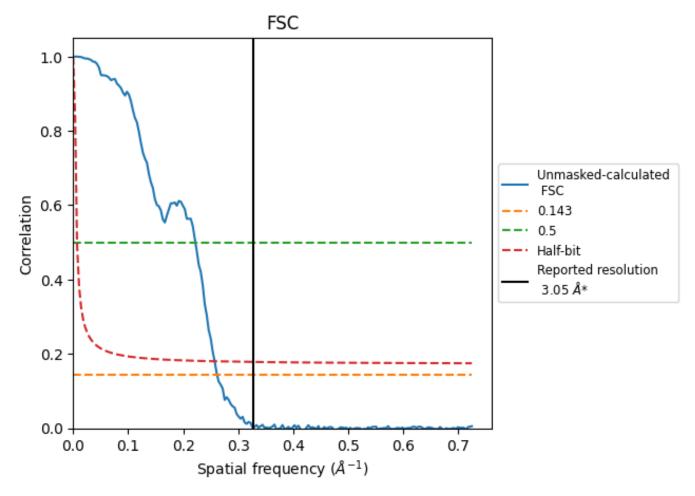
*Reported resolution corresponds to spatial frequency of 0.328 $\mathrm{\AA^{-1}}$



8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.328 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit	
Reported by author	3.05	-	-	
Author-provided FSC curve	-	-	-	
Unmasked-calculated*	3.82	4.50	3.89	

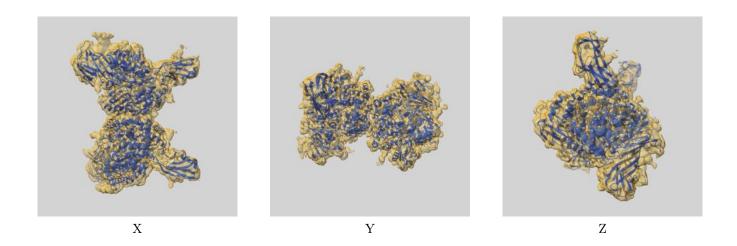
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 3.05 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-39694 and PDB model 8YZI. Per-residue inclusion information can be found in section 3 on page 7.

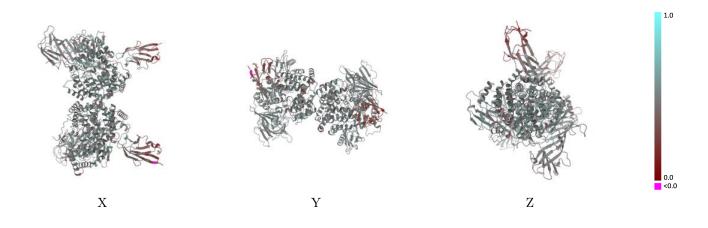
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.141 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.

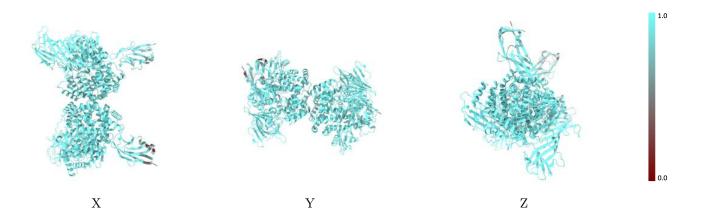


9.2 Q-score mapped to coordinate model (i)



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.

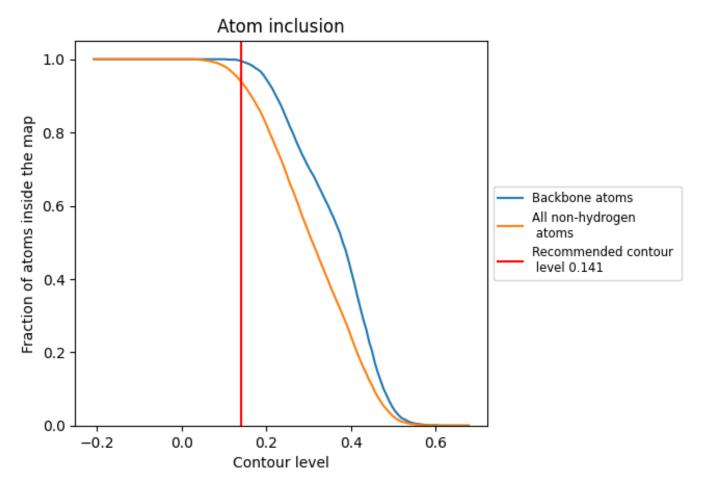
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.141).



9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



Map-model fit summary (i) 9.5

The table lists the average atom inclusion at the recommended contour level (0.141) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9380	0.4830	
А	0.8190	0.3660	1.0
В	0.9550	0.4980	1.0
С	0.8370	0.3550	
D	0.9510	0.5000	
Е	0.8930	0.3950	
F	1.0000	0.4870	
G	0.9200	0.4200	
Н	0.8210	0.4540	
Ι	0.9290	0.4480	
J	0.9640	0.5010	0.0
K	0.9640	0.5080	<0.0
L	0.8930	0.4730]
М	0.8570	0.4300	
N	0.8570	0.3720	

