wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 08:13 AM EST

PDB ID	:	3J2P
EMDB ID	:	EMD-5499
Title	:	CryoEM structure of Dengue virus envelope protein heterotetramer
Authors	:	Zhang, X.; Ge, P.; Yu, X.; Brannan, J.M.; Bi, G.; Zhang, Q.; Schein, S.; Zhou, Z.H.
Deposited on	:	2012-11-30
Resolution	:	3.60 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 ⓘ 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:

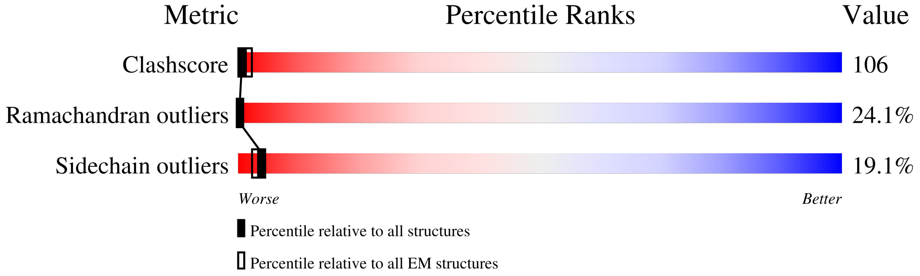
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

1 Overall quality at a glance ⓘ

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

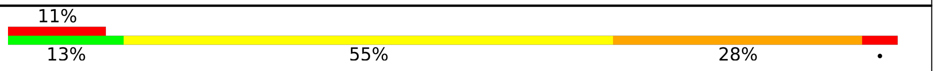
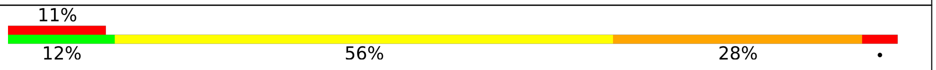
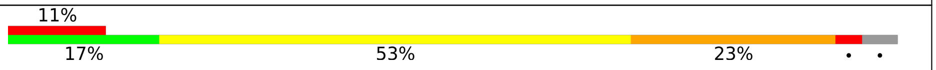
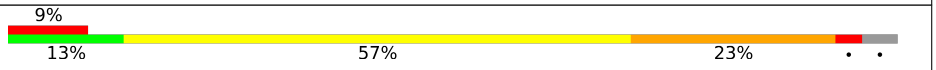
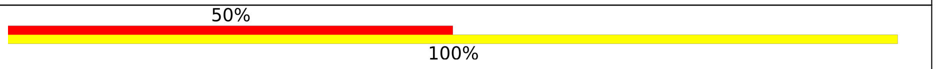
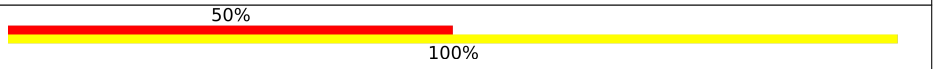
The reported resolution of this entry is 3.60 Å.

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	495	
1	C	495	
2	B	75	
2	D	75	
3	E	2	
3	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9890 atoms, of which 1086 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 Envelope protein E.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	495	Total 4276	C 2410	H 475	N 648	O 711	S 32	0	0
1	C	495	Total 4276	C 2410	H 475	N 648	O 711	S 32	0	0

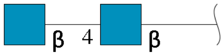
- Molecule 2 is a protein called Small envelope protein M.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	72	Total 627	C 366	H 68	N 95	O 95	S 3	0	0
2	D	72	Total 627	C 366	H 68	N 95	O 95	S 3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ALA	ARG	SEE REMARK 999	UNP P14340
D	15	ALA	ARG	SEE REMARK 999	UNP P14340

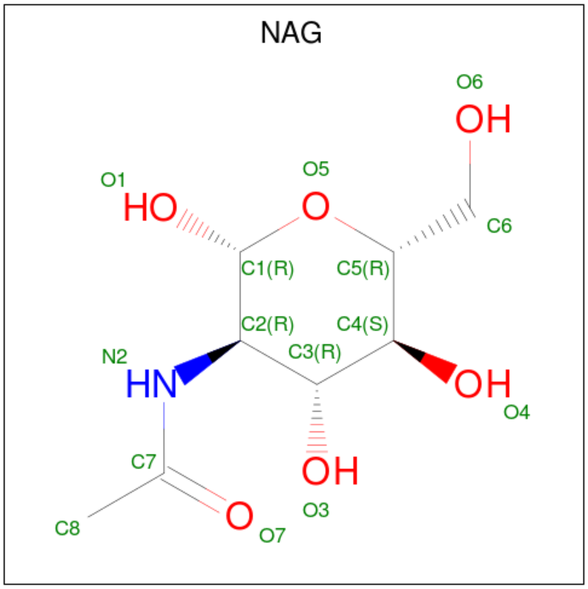
- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0
3	F	2	Total 28	C 16	N 2	O 10	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



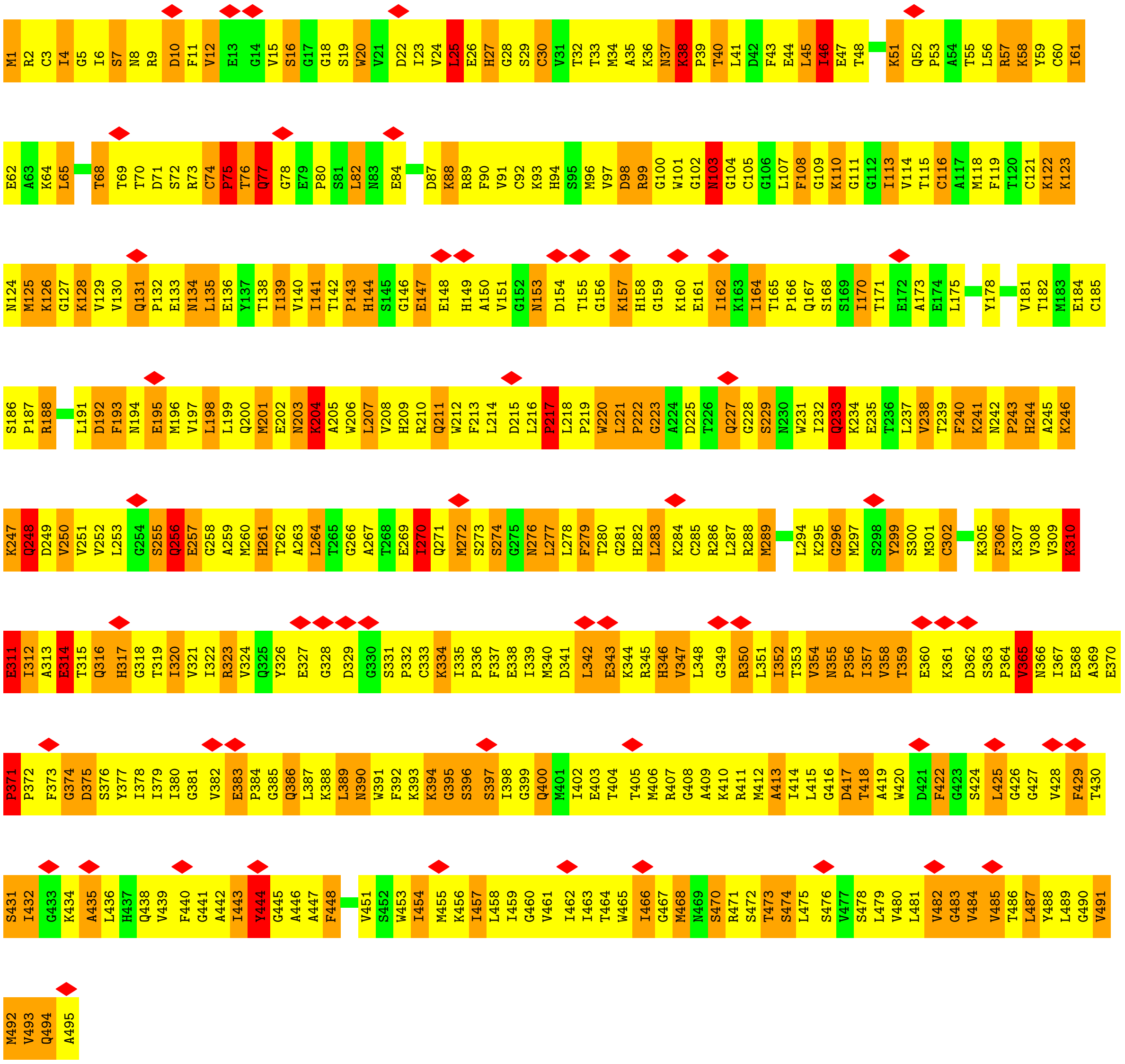
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0

3 Residue-property plots ⓘ

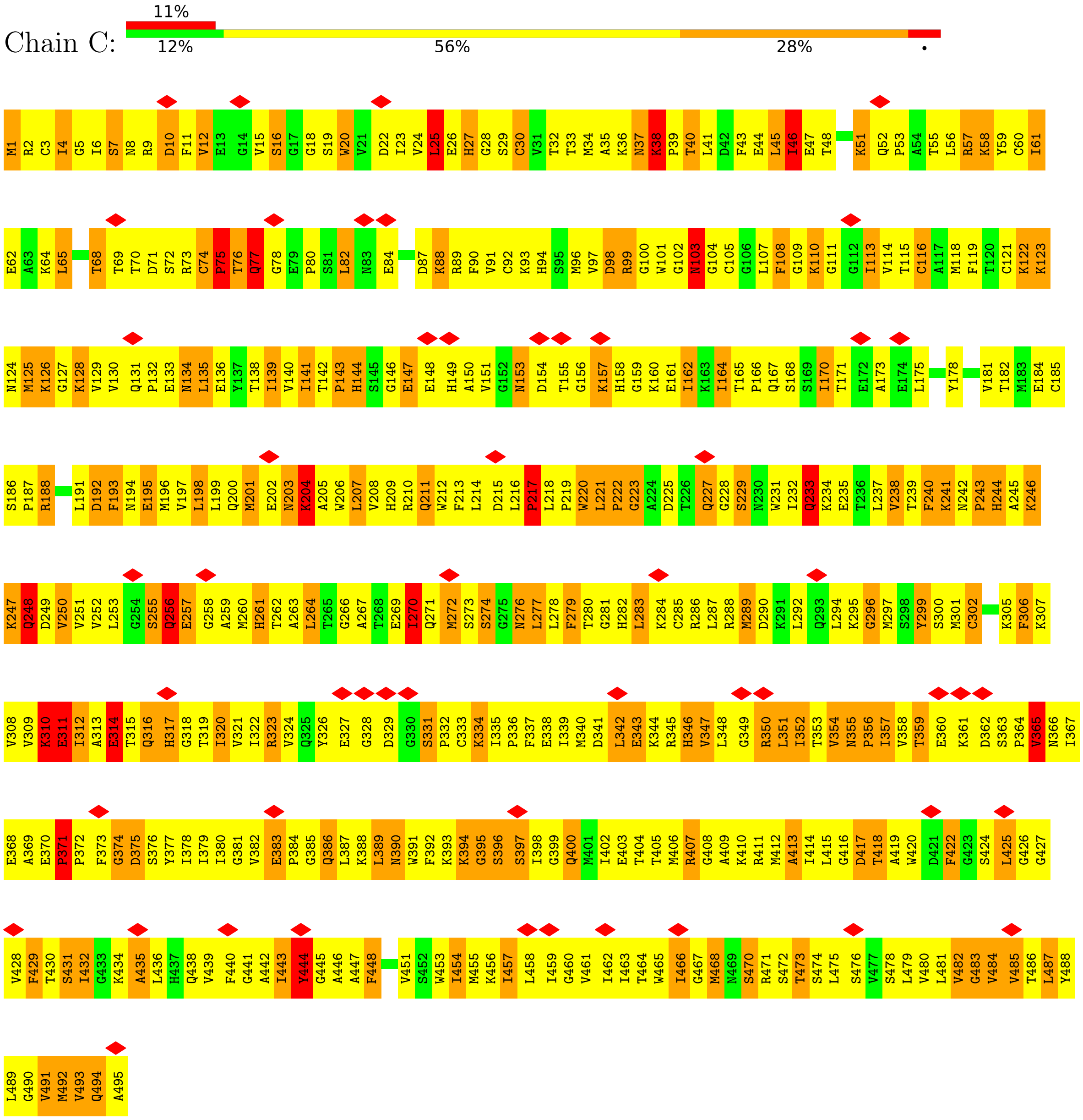
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Envelope protein E

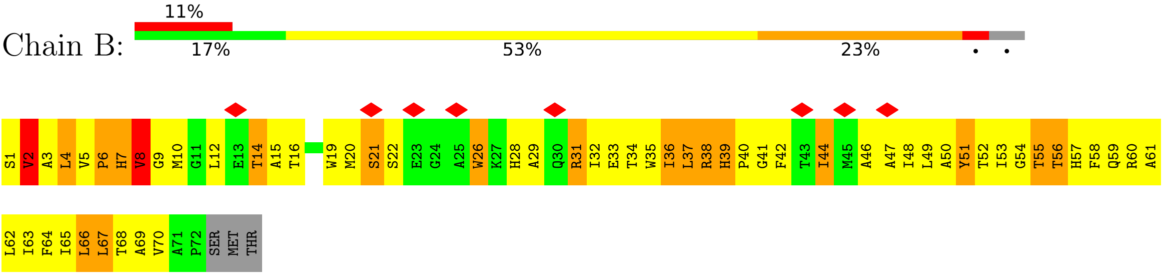
Chain A:



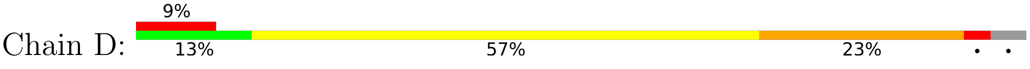
- Molecule 1: Envelope protein E

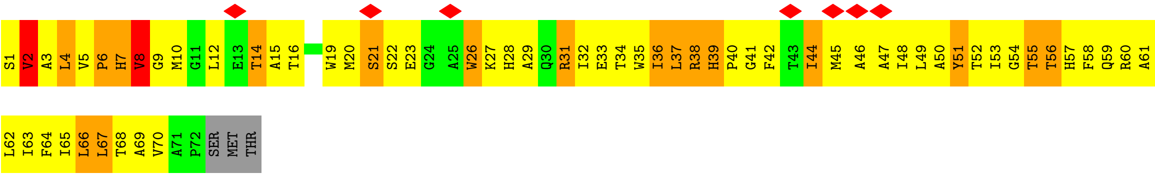


- Molecule 2: Small envelope protein M



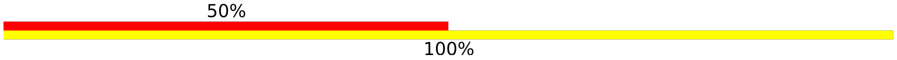
- Molecule 2: Small envelope protein M





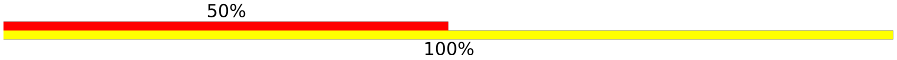
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain F:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9288	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	EMAN, per particle, with astigmatism compensation	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	57518	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	24.021	Depositor
Minimum map value	-17.318	Depositor
Average map value	0.100	Depositor
Map value standard deviation	2.332	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	132.48, 176.64, 132.48	wwPDB
Map dimensions	120, 160, 120	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.104, 1.104, 1.104	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.46	0/3876	0.82	1/5237 (0.0%)
1	C	0.46	0/3876	0.82	1/5237 (0.0%)
2	B	0.49	0/575	0.77	0/786
2	D	0.50	0/575	0.77	0/786
All	All	0.46	0/8902	0.82	2/12046 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	25	LEU	CA-CB-CG	-5.64	102.33	115.30
1	C	25	LEU	CA-CB-CG	-5.56	102.51	115.30

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	3801	475	3844	838	0
1	C	3801	475	3844	820	0
2	B	559	68	569	117	0
2	D	559	68	569	119	0
3	E	28	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	25	3	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
All	All	8804	1086	8902	1831	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 106.

The worst 5 of 1831 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)
2:D:51:TYR:HA	2:D:60:ARG:HD3	1.18	1.17
2:B:51:TYR:HA	2:B:60:ARG:HD3	1.17	1.14
2:B:55:THR:HA	2:B:60:ARG:HH11	1.01	1.14
2:B:55:THR:HA	2:B:60:ARG:NH1	1.65	1.10
2:D:55:THR:HA	2:D:60:ARG:HH11	1.01	1.08

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	493/495 (100%)	228 (46%)	144 (29%)	121 (24%)	0	0
1	C	493/495 (100%)	227 (46%)	144 (29%)	122 (25%)	0	0
2	B	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	1
2	D	70/75 (93%)	33 (47%)	23 (33%)	14 (20%)	0	1
All	All	1126/1140 (99%)	521 (46%)	334 (30%)	271 (24%)	0	0

5 of 271 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	30	CYS
1	A	57	ARG
1	A	74	CYS
1	A	77	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	420/420 (100%)	340 (81%)	80 (19%)	1 9
1	C	420/420 (100%)	340 (81%)	80 (19%)	1 9
2	B	57/60 (95%)	46 (81%)	11 (19%)	1 9
2	D	57/60 (95%)	46 (81%)	11 (19%)	1 9
All	All	954/960 (99%)	772 (81%)	182 (19%)	4 9

5 of 182 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	ILE
1	C	310	LYS
1	C	162	ILE
1	C	241	LYS
1	C	351	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	HIS
1	C	400	GLN
1	C	131	GLN
1	C	256	GLN
1	C	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 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	$\#\|Z\| > 2$
3	NAG	E	1	1,3	14,14,15	0.57	0	17,19,21	0.75	0
3	NAG	E	2	3	14,14,15	0.59	0	17,19,21	0.79	1 (5%)
3	NAG	F	1	1,3	14,14,15	0.59	0	17,19,21	0.74	0
3	NAG	F	2	3	14,14,15	0.58	0	17,19,21	0.78	1 (5%)

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
3	NAG	E	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C2-N2-C7	-2.14	119.86	122.90
3	F	2	NAG	C2-N2-C7	-2.11	119.90	122.90

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C3-C2-N2-C7
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2

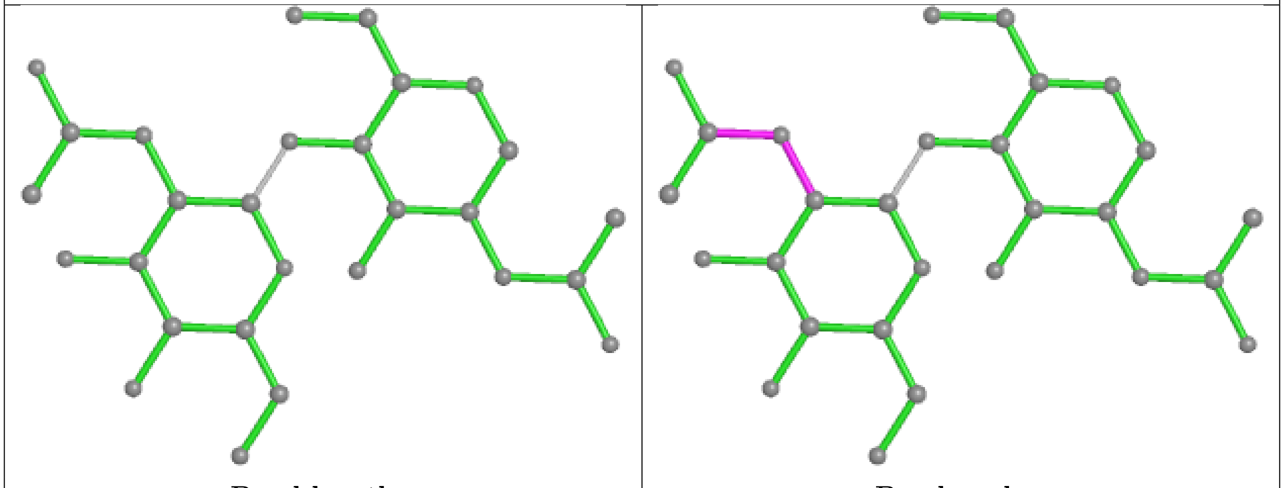
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	3	0
3	F	1	NAG	3	0

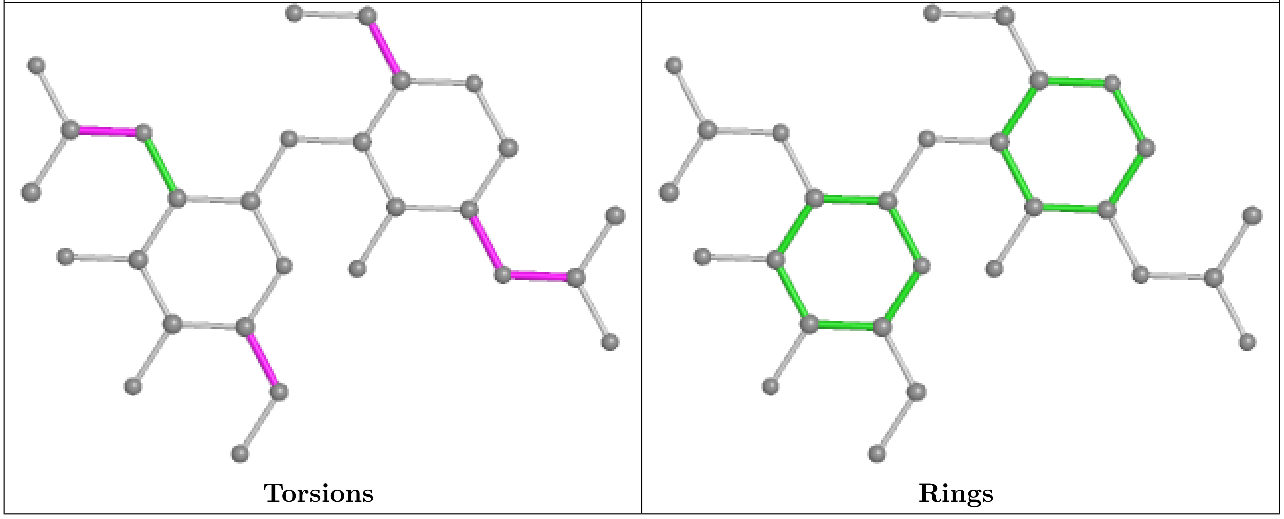
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



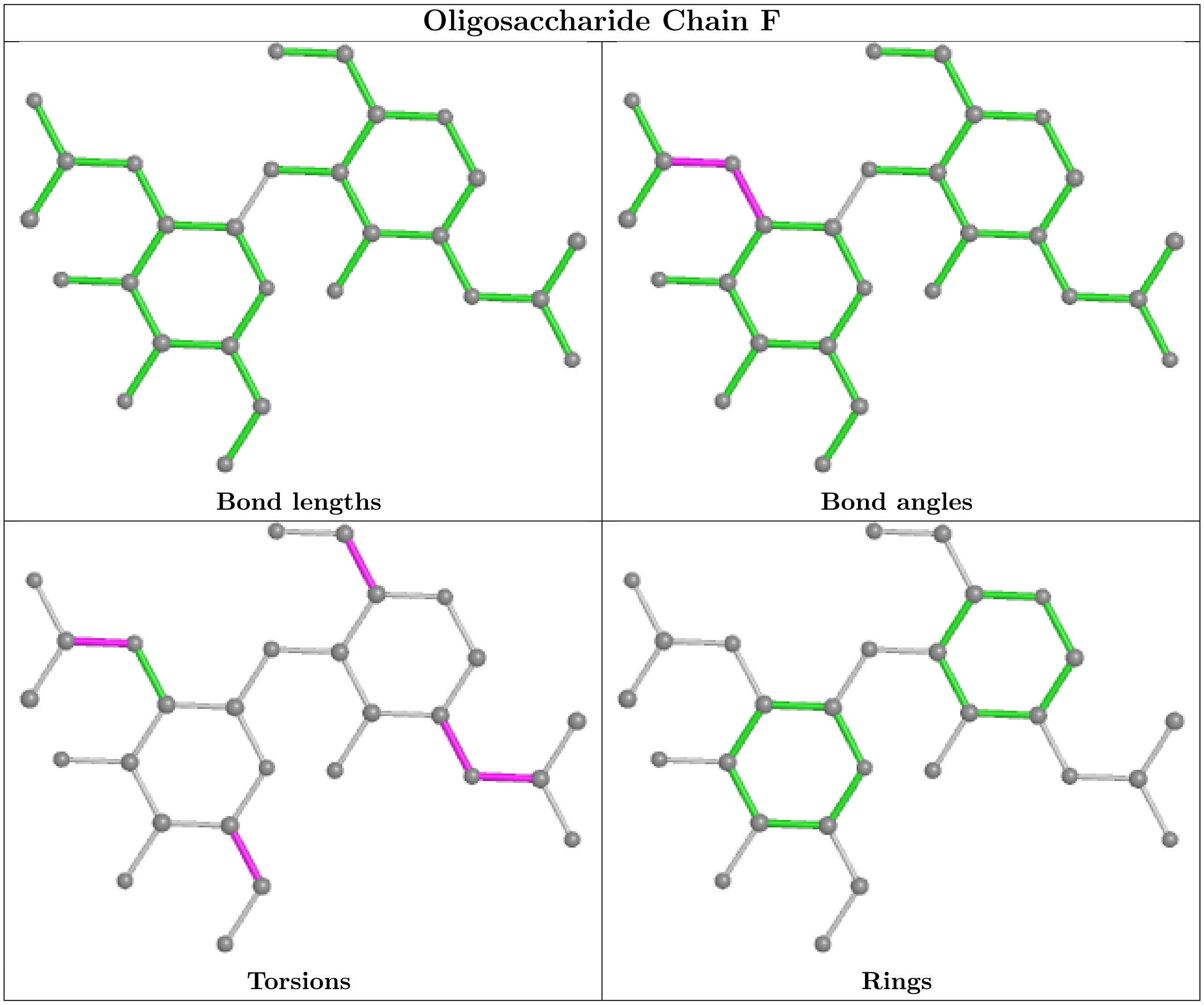
Bond lengths

Bond angles



Torsions

Rings



5.6 Ligand geometry ⓘ

2 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	501	1	14,14,15	0.52	0	17,19,21	0.83	1 (5%)
4	NAG	C	501	1	14,14,15	0.52	0	17,19,21	0.84	1 (5%)

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	A	501	1	-	4/6/23/26	0/1/1/1
4	NAG	C	501	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	NAG	C2-N2-C7	-2.62	119.17	122.90
4	A	501	NAG	C2-N2-C7	-2.58	119.23	122.90

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C8-C7-N2-C2
4	A	501	NAG	O7-C7-N2-C2
4	C	501	NAG	C8-C7-N2-C2
4	C	501	NAG	O7-C7-N2-C2
4	A	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

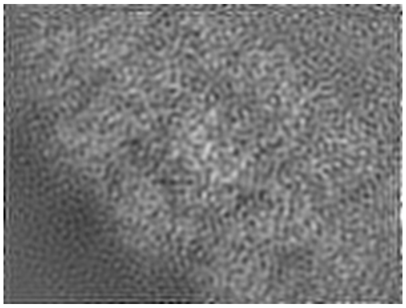
6 Map visualisation

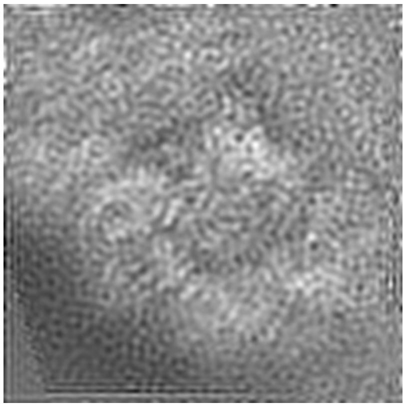
This section contains visualisations of the EMDB entry EMD-5499. These allow visual inspection of the internal detail of the map and identification of artifacts.

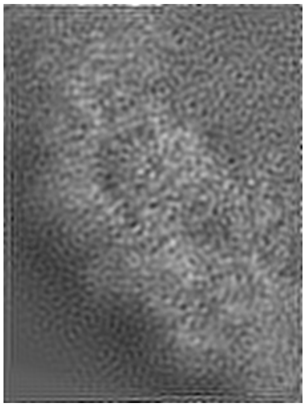
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map


X

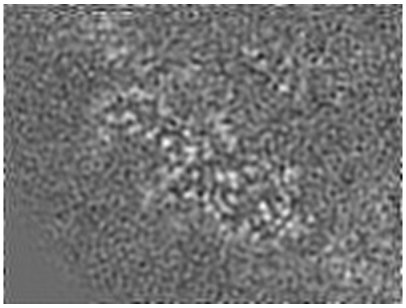

Y

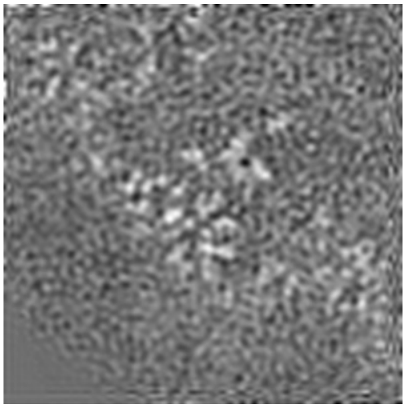

Z

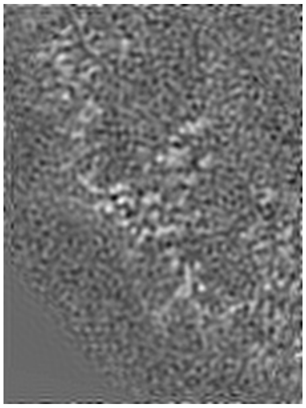
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map


X Index: 60

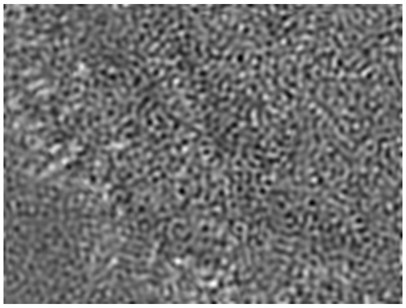

Y Index: 80


Z Index: 60

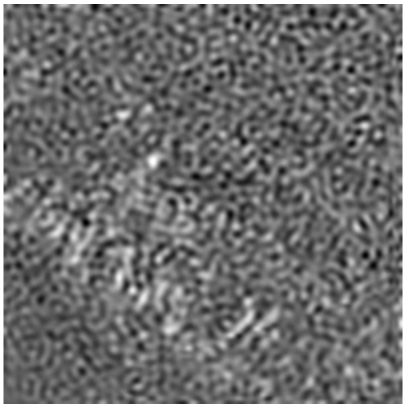
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

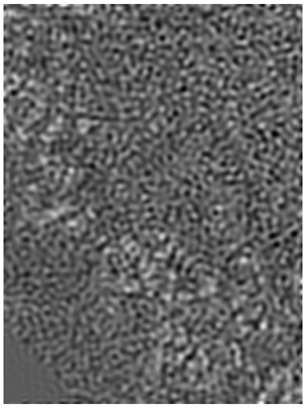
6.3.1 Primary map



X Index: 119



Y Index: 159

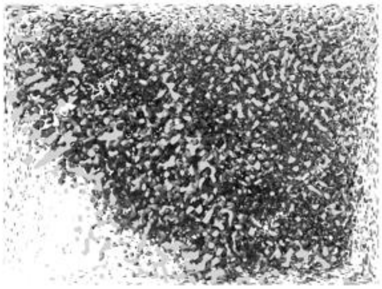


Z Index: 119

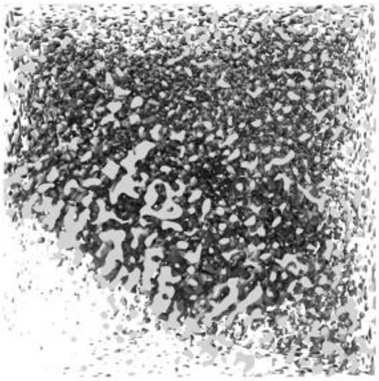
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

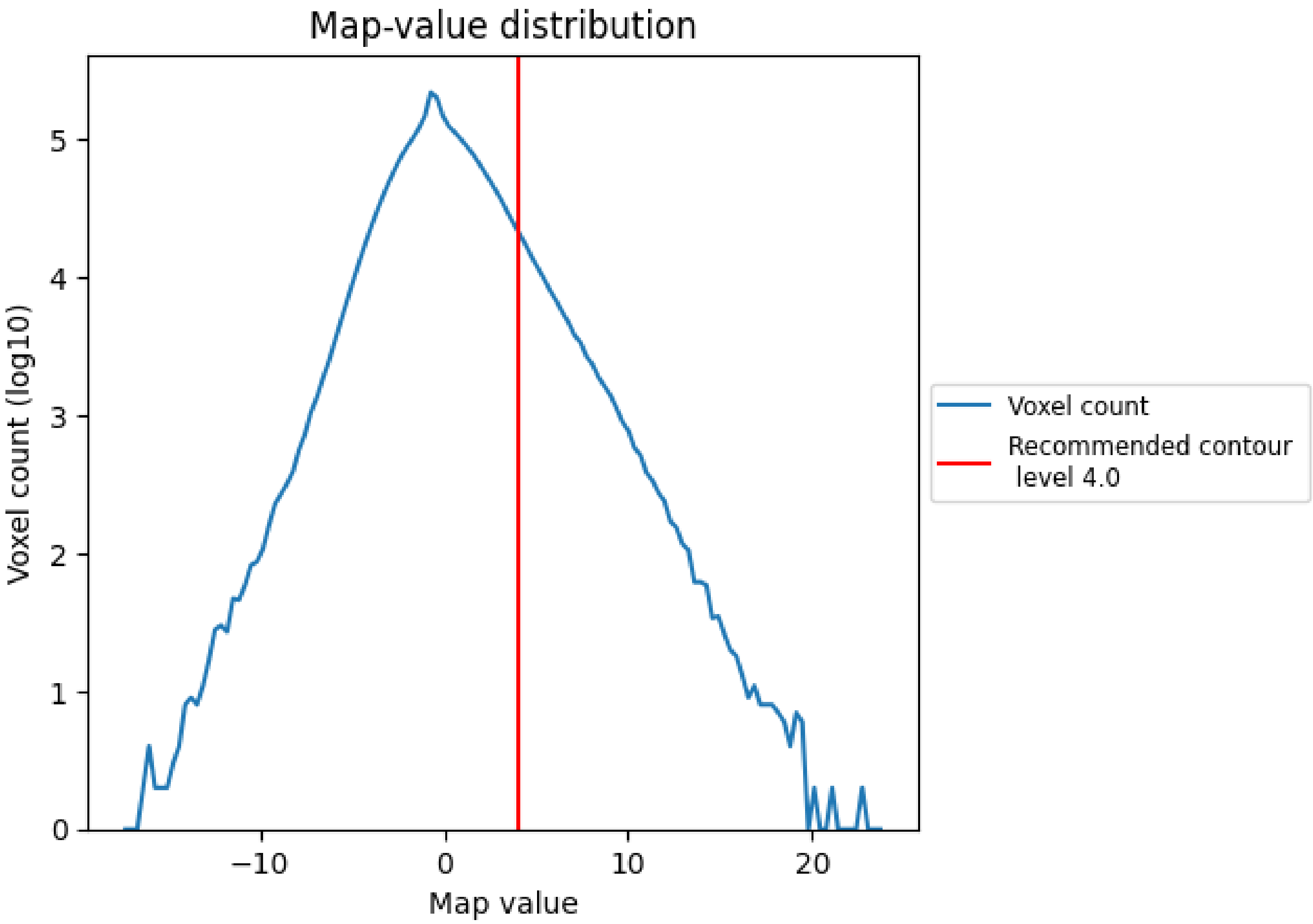
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

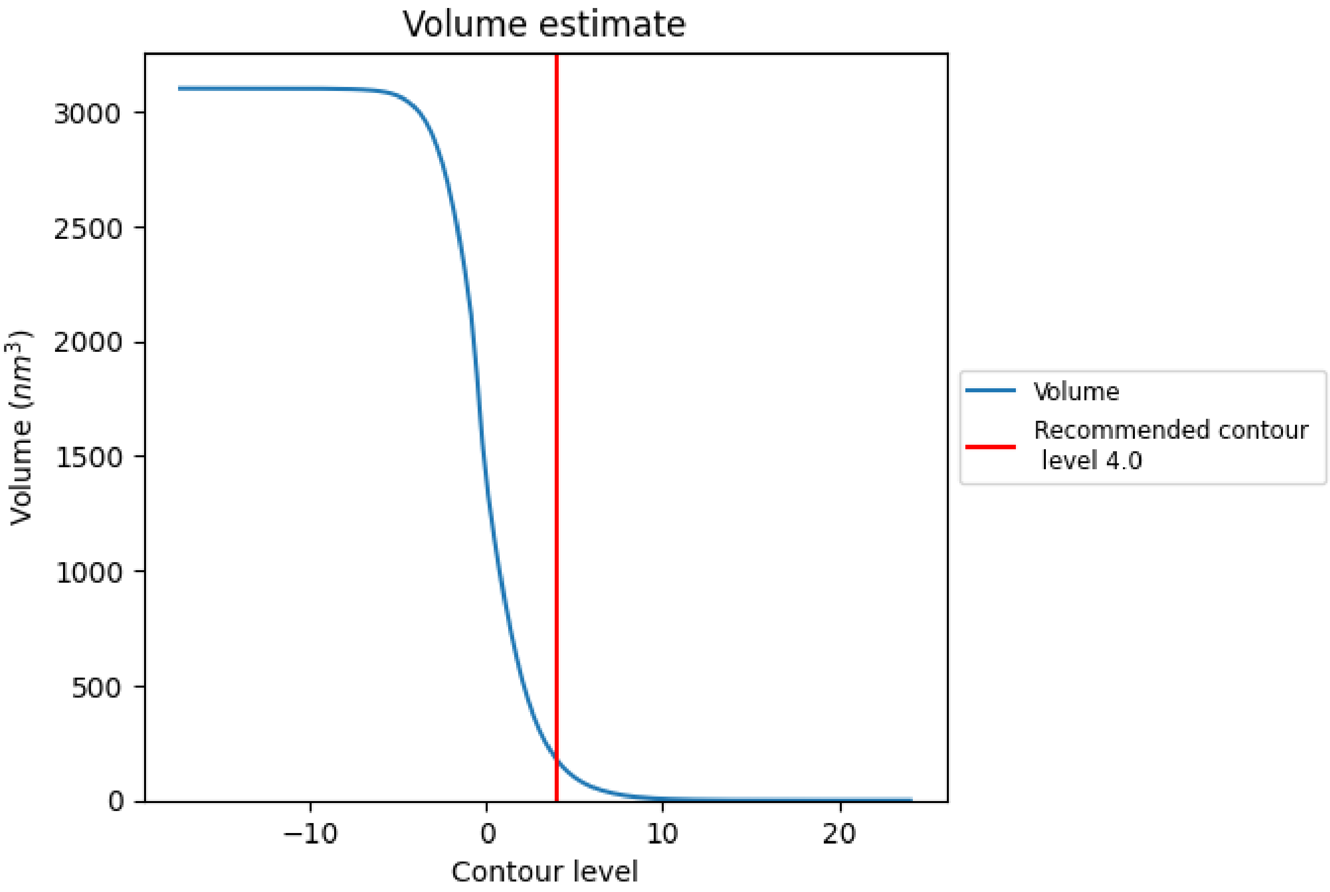
This section contains the results of statistical analysis of the map.

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 177 nm^3; this corresponds to an approximate mass of 160 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 ⓘ

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

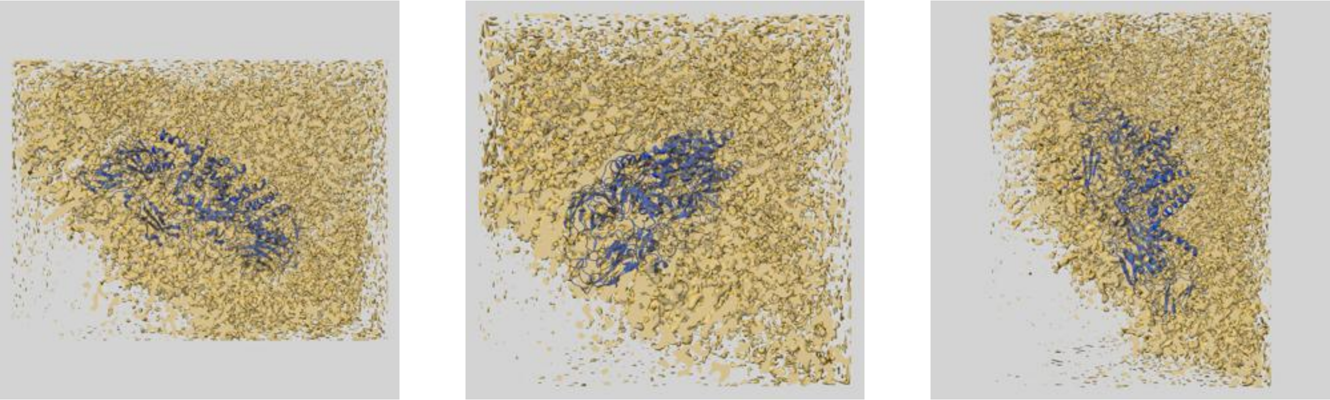
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

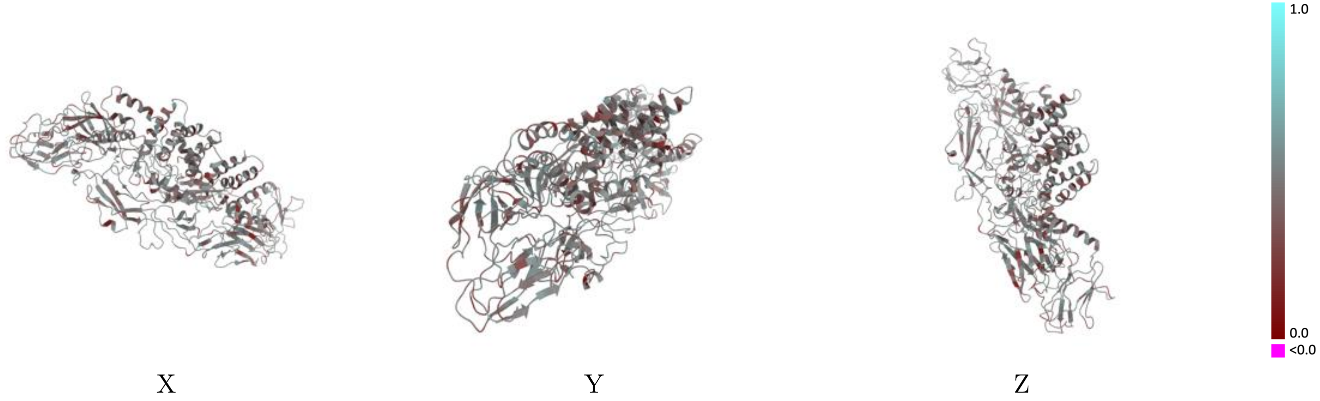
This section contains information regarding the fit between EMDB map EMD-5499 and PDB model 3J2P. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay ⓘ


X Y Z

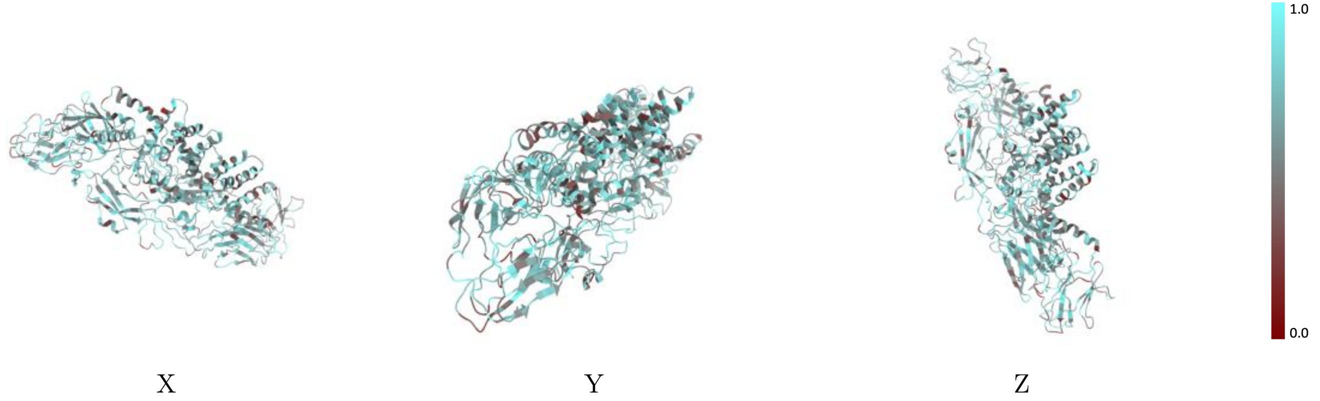
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model



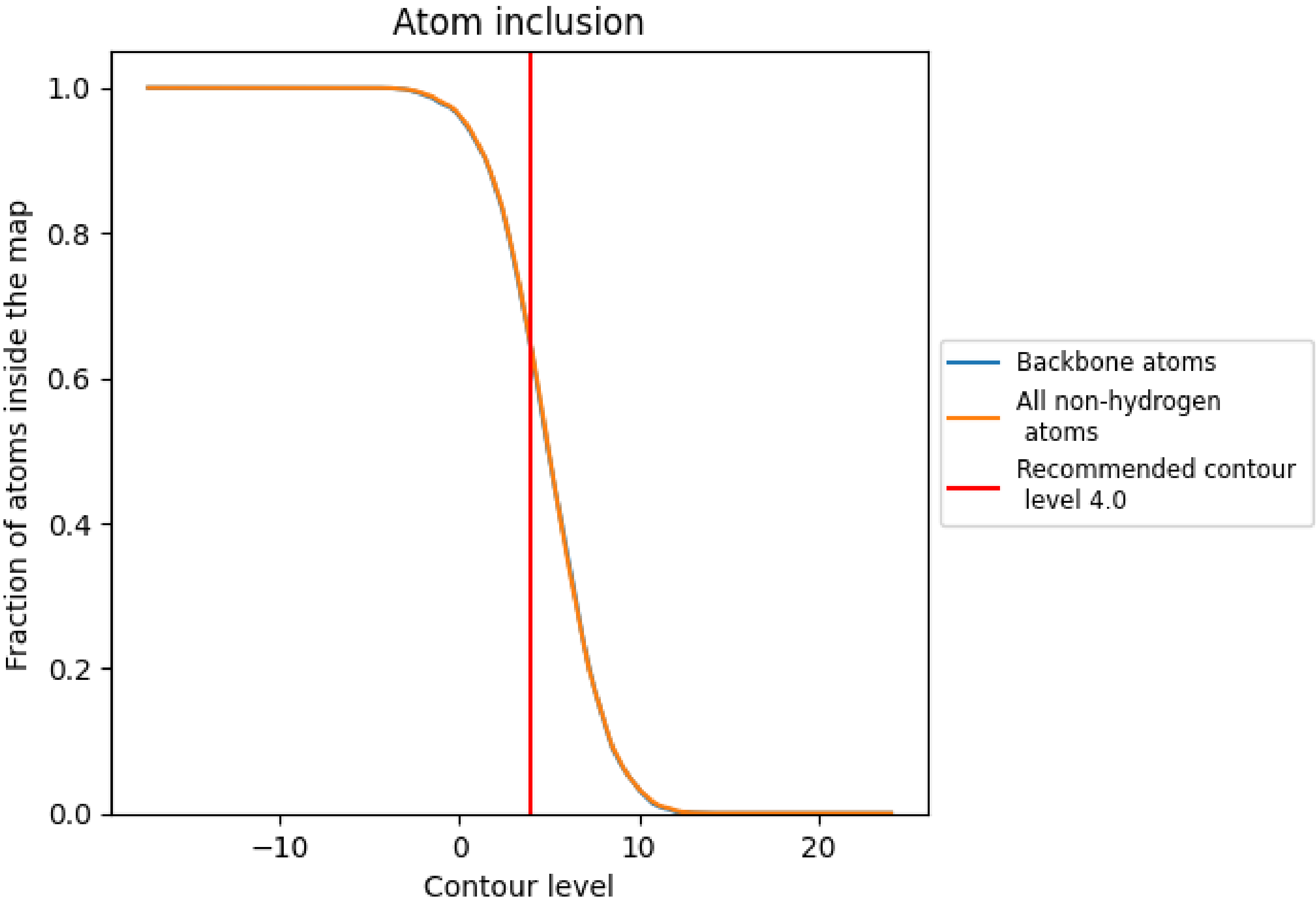
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (4.0).

9.4 Atom inclusion ⓘ



At the recommended contour level, 64% of all backbone atoms, 64% 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 (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6414	0.4450
A	0.6452	0.4450
B	0.6485	0.4450
C	0.6481	0.4450
D	0.6448	0.4460
E	0.3929	0.4390
F	0.4286	0.4420