wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:59 PM EST

PDB ID	:	7N0D
EMDB ID	:	EMD-24104
Title	:	Cryo-EM structure of the tetrameric form of SARS-CoV-2 nsp10-nsp14 (E191A)-RNA complex
Authors	:	Liu, C.; Yang, Y.
Deposited on	:	2021-05-25
Resolution	:	2.50 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:

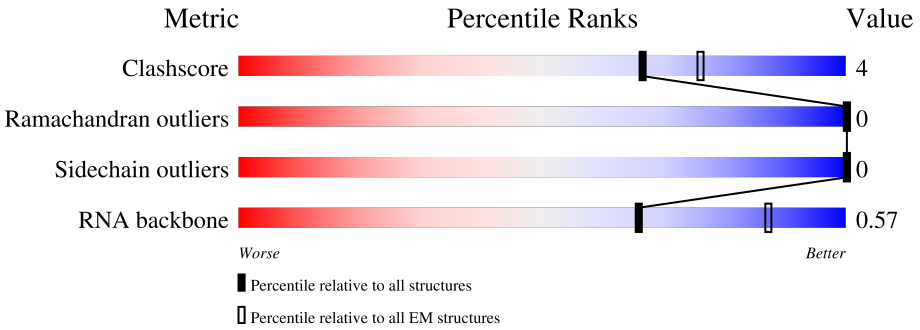
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.50 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
RNA backbone	4643	859

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	139	88% 6% 6%
1	C	139	85% 9% 6%
1	E	139	86% 8% 6%
1	G	139	85% 9% 6%
2	B	527	90% 7%
2	D	527	85% 12%
2	F	527	90% 7%

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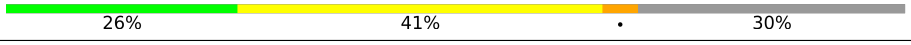
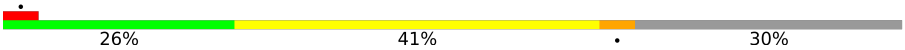
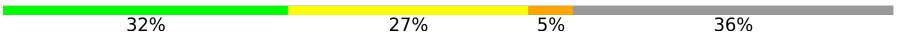
Mol	Chain	Length	Quality of chain
2	H	527	
3	I	27	
3	T	27	
4	K	22	
4	L	22	
5	J	5	
5	P	5	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 21846 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	131	Total	C	N	O	S	0	0
			955	593	160	186	16		
1	C	131	Total	C	N	O	S	0	0
			955	593	160	186	16		
1	E	131	Total	C	N	O	S	0	0
			955	593	160	186	16		
1	G	131	Total	C	N	O	S	0	0
			955	593	160	186	16		

- Molecule 2 is a protein called Proofreading exoribonuclease.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	512	Total	C	N	O	S	0	0
			4085	2624	694	731	36		
2	D	512	Total	C	N	O	S	0	0
			4085	2624	694	731	36		
2	F	512	Total	C	N	O	S	0	0
			4085	2624	694	731	36		
2	H	512	Total	C	N	O	S	0	0
			4085	2624	694	731	36		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	191	ALA	GLU	engineered mutation	UNP P0DTD1
D	191	ALA	GLU	engineered mutation	UNP P0DTD1
F	191	ALA	GLU	engineered mutation	UNP P0DTD1
H	191	ALA	GLU	engineered mutation	UNP P0DTD1

- Molecule 3 is a RNA chain called RNA (5'-R(*GP*GP*GP*GP*AP*UP*GP*UP*GP*AP*UP*UP*UP*UP*AP*AP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	19	Total	C	N	O	P	0	0
			411	183	74	135	19		
3	I	19	Total	C	N	O	P	0	0
			411	183	74	135	19		

- Molecule 4 is a RNA chain called RNA (5'-R(*CP*UP*AP*UP*UP*AP*AP*AP*AP*UP*CP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	14	Total	C	N	O	P	0	0
			292	132	50	96	14		
4	L	14	Total	C	N	O	P	0	0
			292	132	50	96	14		

- Molecule 5 is a RNA chain called RNA (5'-R(*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	5	Total	C	N	O	P	0	0
			100	45	15	35	5		
5	J	5	Total	C	N	O	P	0	0
			100	45	15	35	5		

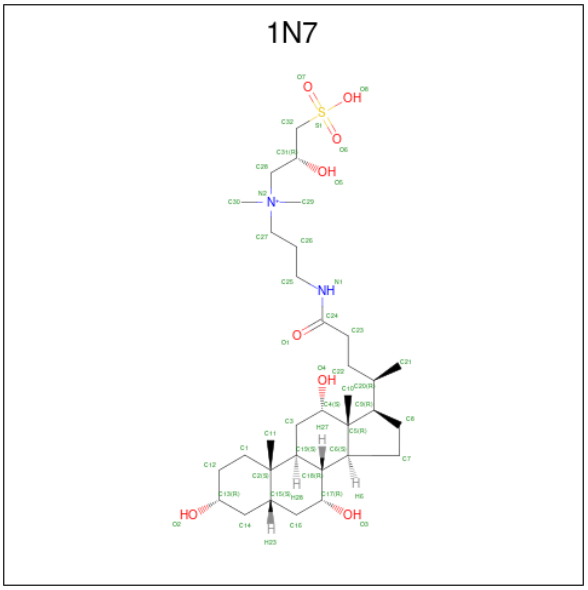
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Zn	0
			2	2	
6	B	3	Total	Zn	0
			3	3	
6	C	2	Total	Zn	0
			2	2	
6	D	3	Total	Zn	0
			3	3	
6	E	2	Total	Zn	0
			2	2	
6	F	3	Total	Zn	0
			3	3	
6	G	2	Total	Zn	0
			2	2	
6	H	3	Total	Zn	0
			3	3	

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
7	B	2	Total Mg 2 2	0
7	D	1	Total Mg 1 1	0
7	F	2	Total Mg 2 2	0
7	H	1	Total Mg 1 1	0

- Molecule 8 is CHAPSO (three-letter code: 1N7) (formula: $C_{32}H_{59}N_2O_8S$).



Mol	Chain	Residues	Atoms	AltConf
8	D	1	Total C O 25 22 3	0
8	H	1	Total C O 25 22 3	0

- Molecule 9 is water.

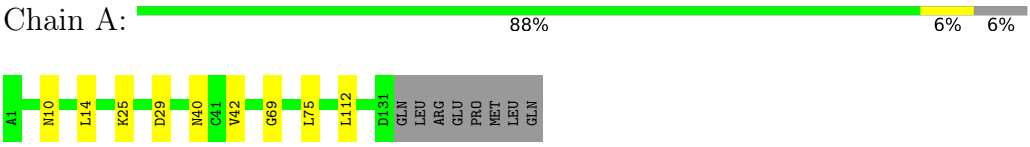
Mol	Chain	Residues	Atoms	AltConf
9	B	1	Total O 1 1	0
9	D	1	Total O 1 1	0
9	F	1	Total O 1 1	0
9	H	1	Total O 1 1	0

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.

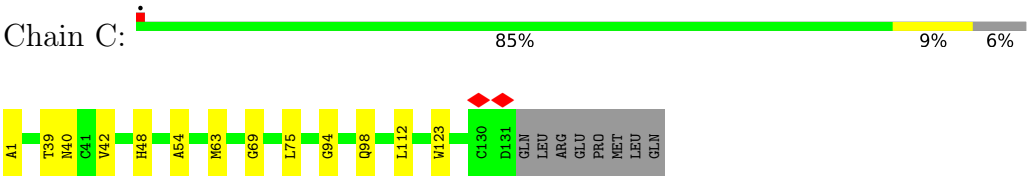
• Molecule 1: Non-structural protein 10

Chain A:



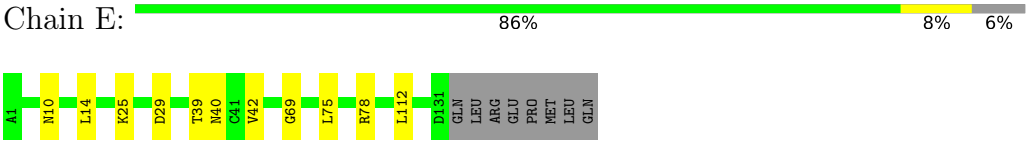
• Molecule 1: Non-structural protein 10

Chain C:



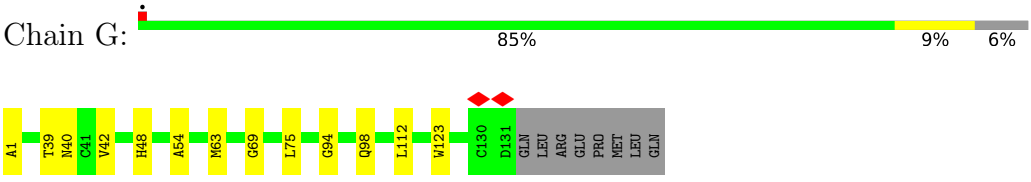
• Molecule 1: Non-structural protein 10

Chain E:



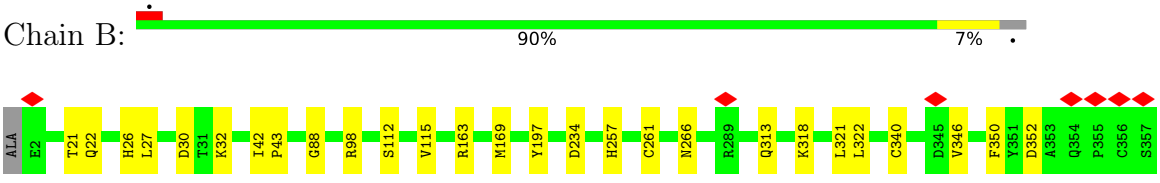
• Molecule 1: Non-structural protein 10

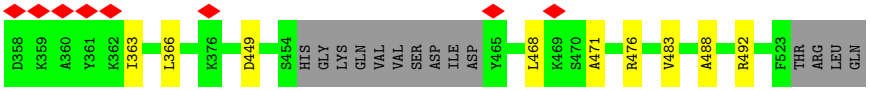
Chain G:



• Molecule 2: Proofreading exoribonuclease

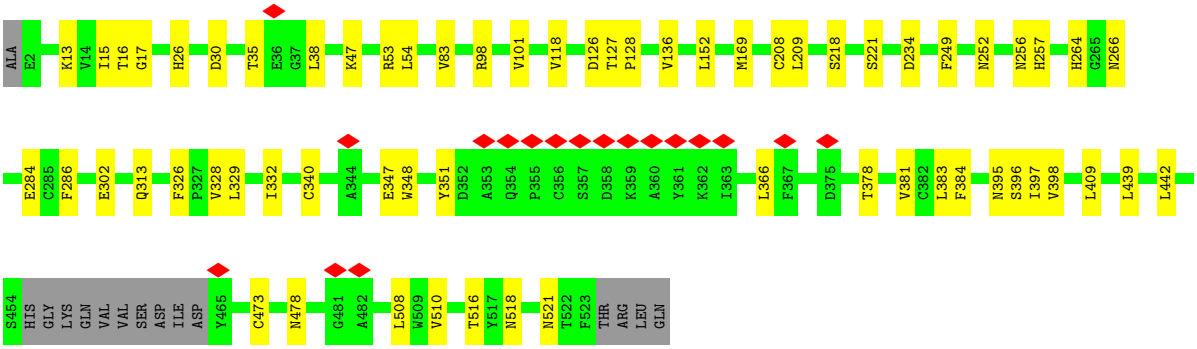
Chain B:





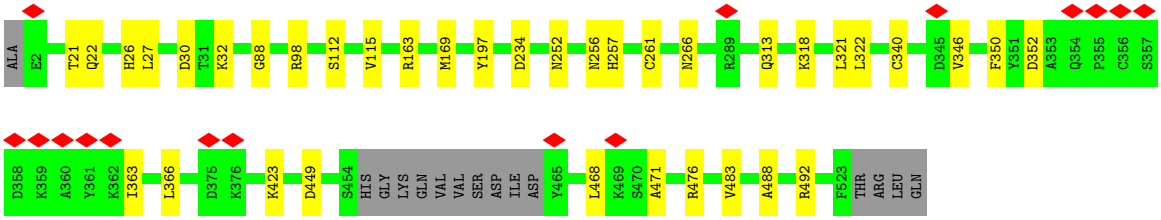
• Molecule 2: Proofreading exoribonuclease

Chain D:



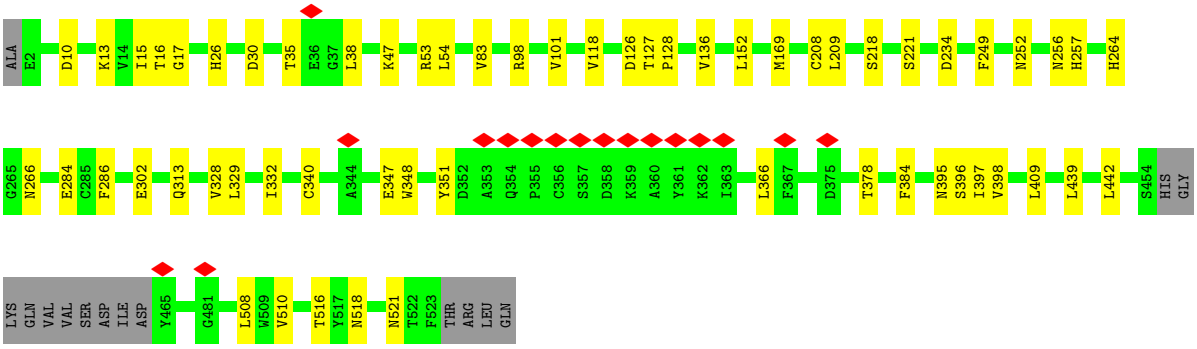
• Molecule 2: Proofreading exoribonuclease

Chain F:



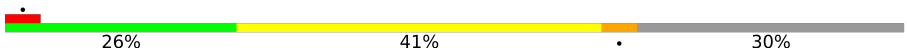
• Molecule 2: Proofreading exoribonuclease

Chain H:



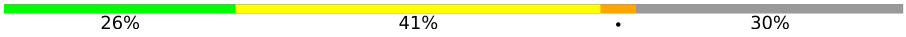
• Molecule 3: RNA (5'-R(*GP*GP*GP*GP*AP*UP*GP*UP*GP*AP*UP*UP*UP*UP*AP*AP *UP*AP*G)-3')

Chain T:



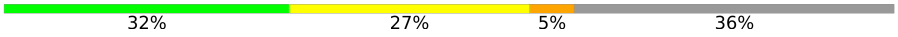
• Molecule 3: RNA (5'-R(*GP*GP*GP*GP*AP*UP*GP*UP*GP*AP*UP*UP*UP*UP*AP*AP*UP*AP*G)-3')

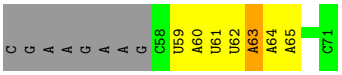
Chain I:



• Molecule 4: RNA (5'-R(*CP*UP*AP*UP*UP*AP*AP*AP*AP*UP*CP*AP*CP*C)-3')

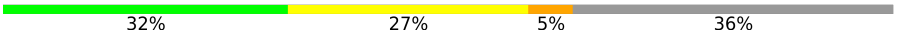
Chain K:

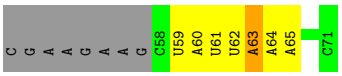




• Molecule 4: RNA (5'-R(*CP*UP*AP*UP*UP*AP*AP*AP*AP*UP*CP*AP*CP*C)-3')

Chain L:





• Molecule 5: RNA (5'-R(*CP*CP*CP*CP*C)-3')

Chain P:

• Molecule 5: RNA (5'-R(*CP*CP*CP*CP*C)-3')

Chain J:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	42228	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 ($e^-/Å^2$)	49.19	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.454	Depositor
Minimum map value	-1.890	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.433	Depositor
Map size (Å)	346.03198, 346.03198, 346.03198	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1N7, MG

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	0.35	0/976	0.55	0/1327
1	C	0.33	0/976	0.57	0/1327
1	E	0.35	0/976	0.55	0/1327
1	G	0.33	0/976	0.56	0/1327
2	B	0.34	0/4203	0.51	0/5715
2	D	0.33	0/4203	0.53	0/5715
2	F	0.34	0/4203	0.51	0/5715
2	H	0.32	0/4203	0.52	0/5715
3	I	0.38	0/460	0.94	0/716
3	T	0.38	0/460	0.94	0/716
4	K	0.34	0/325	0.94	0/502
4	L	0.35	0/325	0.94	0/502
5	J	0.39	0/109	0.75	0/166
5	P	0.40	0/109	0.75	0/166
All	All	0.34	0/22504	0.57	0/30936

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

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	955	0	910	6	0
1	C	955	0	910	12	0
1	E	955	0	910	7	0
1	G	955	0	910	12	0
2	B	4085	0	3966	21	0
2	D	4085	0	3966	42	0
2	F	4085	0	3966	22	0
2	H	4085	0	3966	39	0
3	I	411	0	203	5	0
3	T	411	0	203	5	0
4	K	292	0	151	5	0
4	L	292	0	151	5	0
5	J	100	0	56	1	0
5	P	100	0	56	1	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	0	0
6	E	2	0	0	0	0
6	F	3	0	0	0	0
6	G	2	0	0	0	0
6	H	3	0	0	0	0
7	B	2	0	0	0	0
7	D	1	0	0	0	0
7	F	2	0	0	0	0
7	H	1	0	0	0	0
8	D	25	0	35	1	0
8	H	25	0	35	1	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
9	F	1	0	0	0	0
9	H	1	0	0	0	0
All	All	21846	0	20394	167	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 4.

The worst 5 of 167 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:127:THR:HG23	2:D:128:PRO:HD2	1.65	0.78
2:D:127:THR:CG2	2:D:128:PRO:HD2	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:THR:HG23	2:H:128:PRO:HD2	1.64	0.77
2:H:127:THR:CG2	2:H:128:PRO:HD2	2.14	0.76
1:G:39:THR:HG22	1:G:40:ASN:N	2.08	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	129/139 (93%)	129 (100%)	0	0	100	100
1	C	129/139 (93%)	127 (98%)	2 (2%)	0	100	100
1	E	129/139 (93%)	129 (100%)	0	0	100	100
1	G	129/139 (93%)	127 (98%)	2 (2%)	0	100	100
2	B	508/527 (96%)	504 (99%)	4 (1%)	0	100	100
2	D	508/527 (96%)	500 (98%)	8 (2%)	0	100	100
2	F	508/527 (96%)	504 (99%)	4 (1%)	0	100	100
2	H	508/527 (96%)	500 (98%)	8 (2%)	0	100	100
All	All	2548/2664 (96%)	2520 (99%)	28 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/113 (93%)	105 (100%)	0	100	100
1	C	105/113 (93%)	105 (100%)	0	100	100
1	E	105/113 (93%)	105 (100%)	0	100	100
1	G	105/113 (93%)	105 (100%)	0	100	100
2	B	448/461 (97%)	448 (100%)	0	100	100
2	D	448/461 (97%)	448 (100%)	0	100	100
2	F	448/461 (97%)	448 (100%)	0	100	100
2	H	448/461 (97%)	448 (100%)	0	100	100
All	All	2212/2296 (96%)	2212 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	313	GLN
2	H	246	GLN
2	H	22	GLN
2	H	313	GLN
2	D	246	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	I	18/27 (66%)	6 (33%)	0
3	T	18/27 (66%)	6 (33%)	0
4	K	13/22 (59%)	1 (7%)	0
4	L	13/22 (59%)	1 (7%)	0
5	J	4/5 (80%)	0	0
5	P	4/5 (80%)	0	0
All	All	70/108 (64%)	14 (20%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	3	G
3	T	9	G
3	T	13	U
3	T	15	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	T	16	A

There are no RNA pucker outliers to report.

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 26 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	1N7	D	605	-	28,28,46	0.76	1 (3%)	46,46,72	1.74	7 (15%)
8	1N7	H	701	-	28,28,46	0.76	1 (3%)	46,46,72	1.74	7 (15%)

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
8	1N7	D	605	-	-	4/4/69/92	0/4/4/4
8	1N7	H	701	-	-	4/4/69/92	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	701	1N7	O4-C4	-2.03	1.40	1.43
8	D	605	1N7	O4-C4	-2.02	1.40	1.43

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	701	1N7	C5-C9-C20	-5.98	112.34	119.49
8	D	605	1N7	C5-C9-C20	-5.93	112.40	119.49
8	D	605	1N7	C3-C19-C2	-4.32	109.27	113.73
8	H	701	1N7	C3-C19-C2	-4.26	109.33	113.73
8	H	701	1N7	C5-C6-C18	-3.88	109.78	114.74

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	605	1N7	C21-C20-C9-C5
8	D	605	1N7	C22-C20-C9-C5
8	D	605	1N7	C21-C20-C9-C8
8	D	605	1N7	C22-C20-C9-C8
8	H	701	1N7	C21-C20-C9-C5

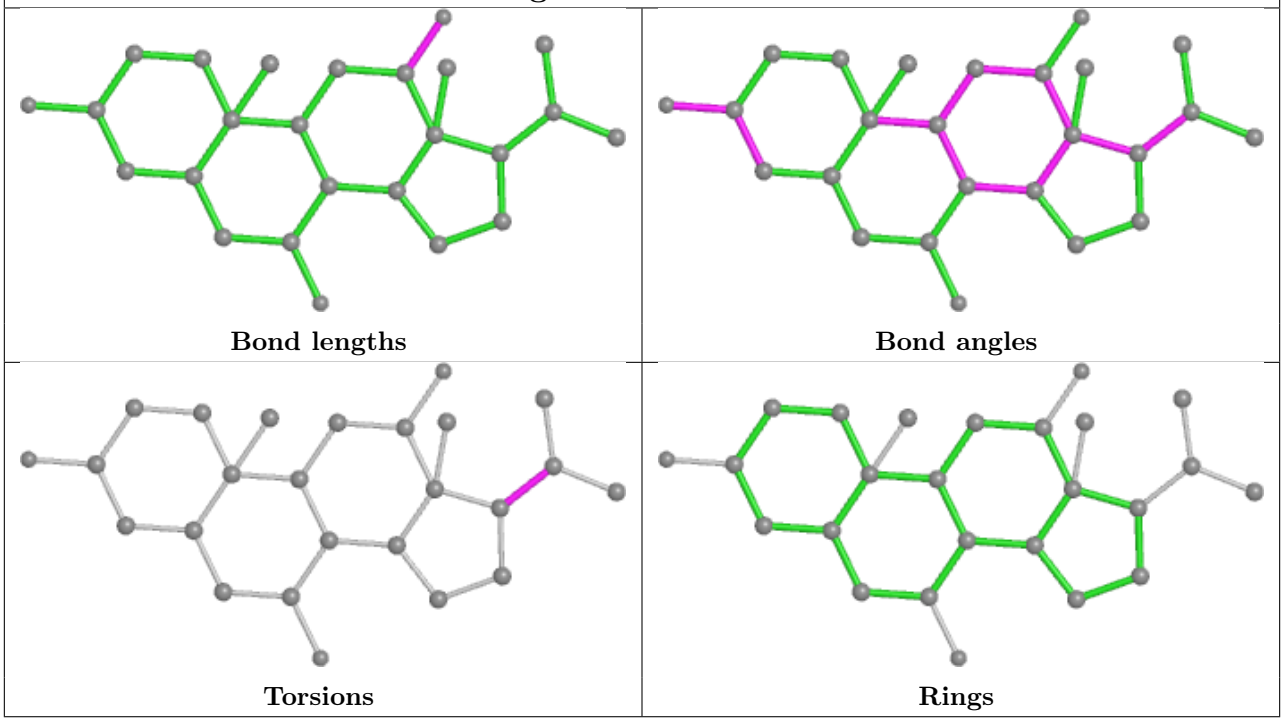
There are no ring outliers.

2 monomers are involved in 2 short contacts:

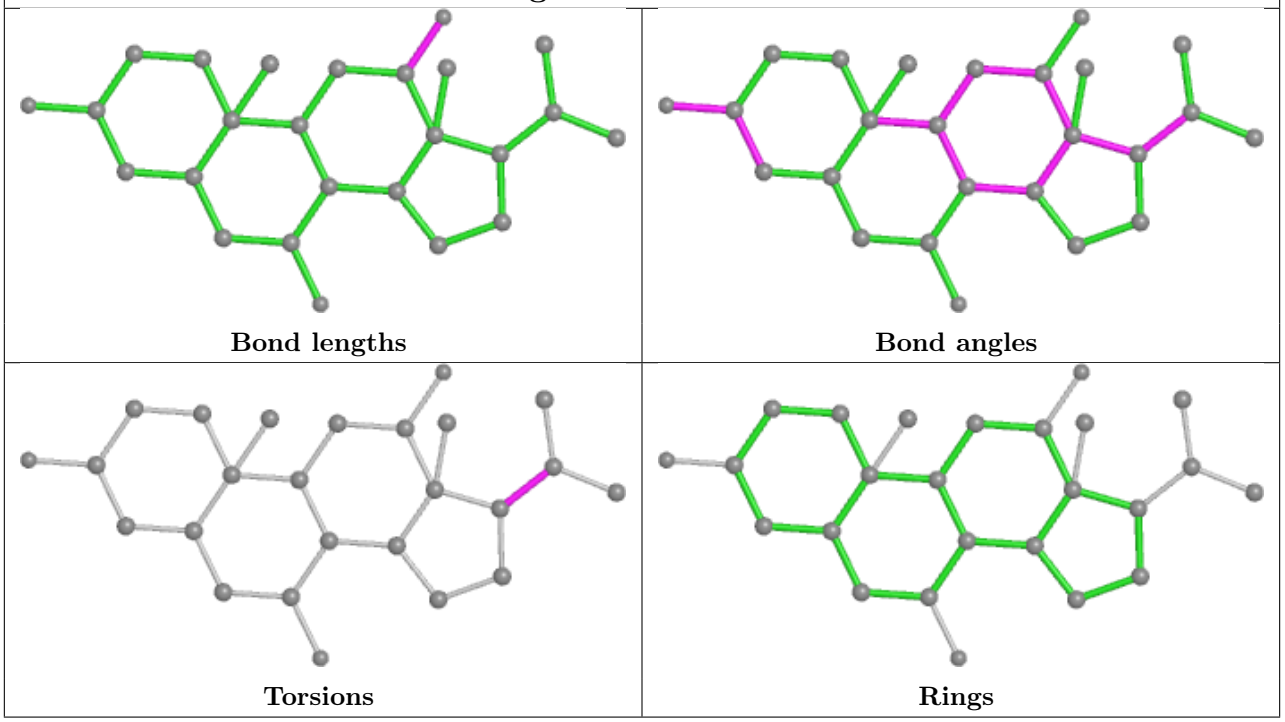
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	605	1N7	1	0
8	H	701	1N7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 1N7 D 605



Ligand 1N7 H 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

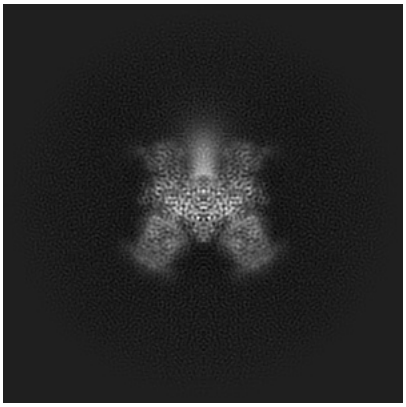
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24104. These allow visual inspection of the internal detail of the map and identification of artifacts.

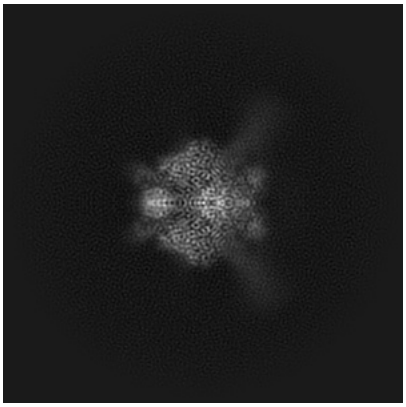
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

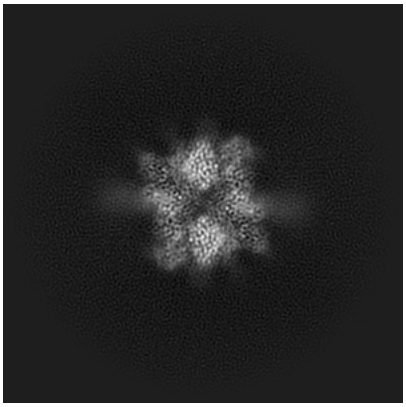
6.1.1 Primary map



X



Y

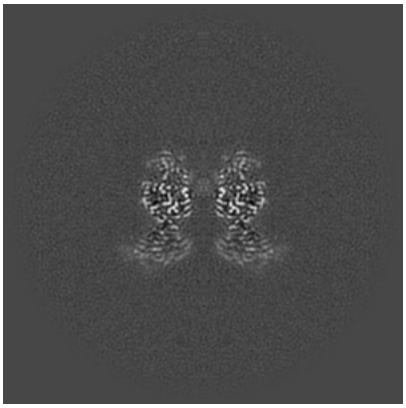


Z

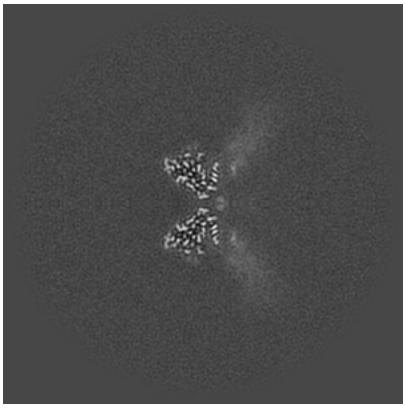
The images above show the map projected in three orthogonal directions.

6.2 Central slices

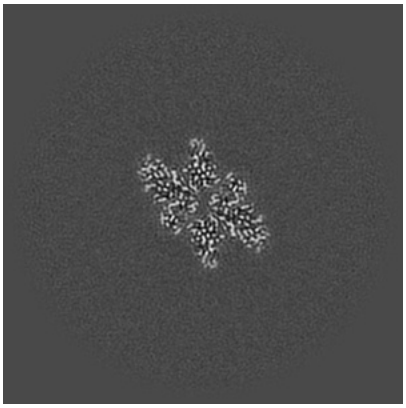
6.2.1 Primary map



X Index: 162



Y Index: 162

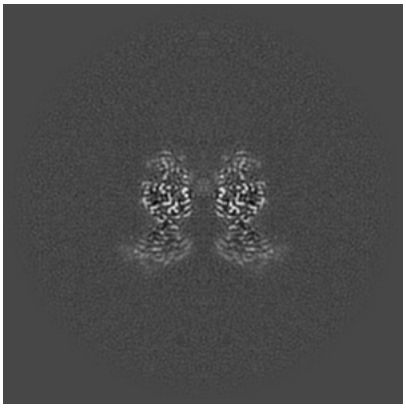


Z Index: 162

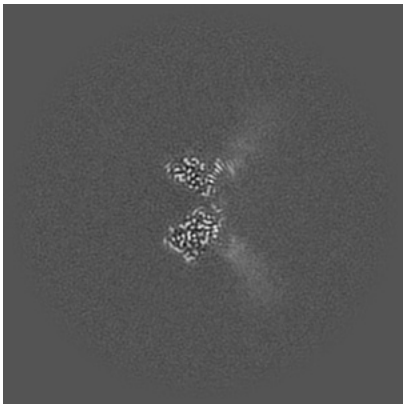
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

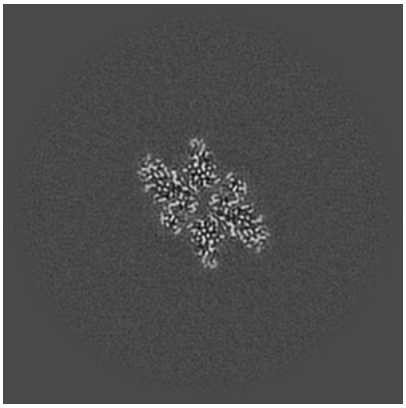
6.3.1 Primary map



X Index: 162



Y Index: 166



Z Index: 162

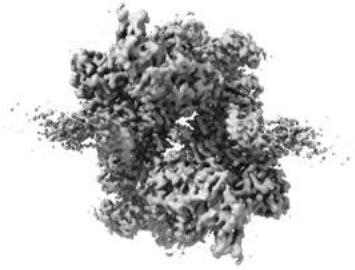
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.433. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

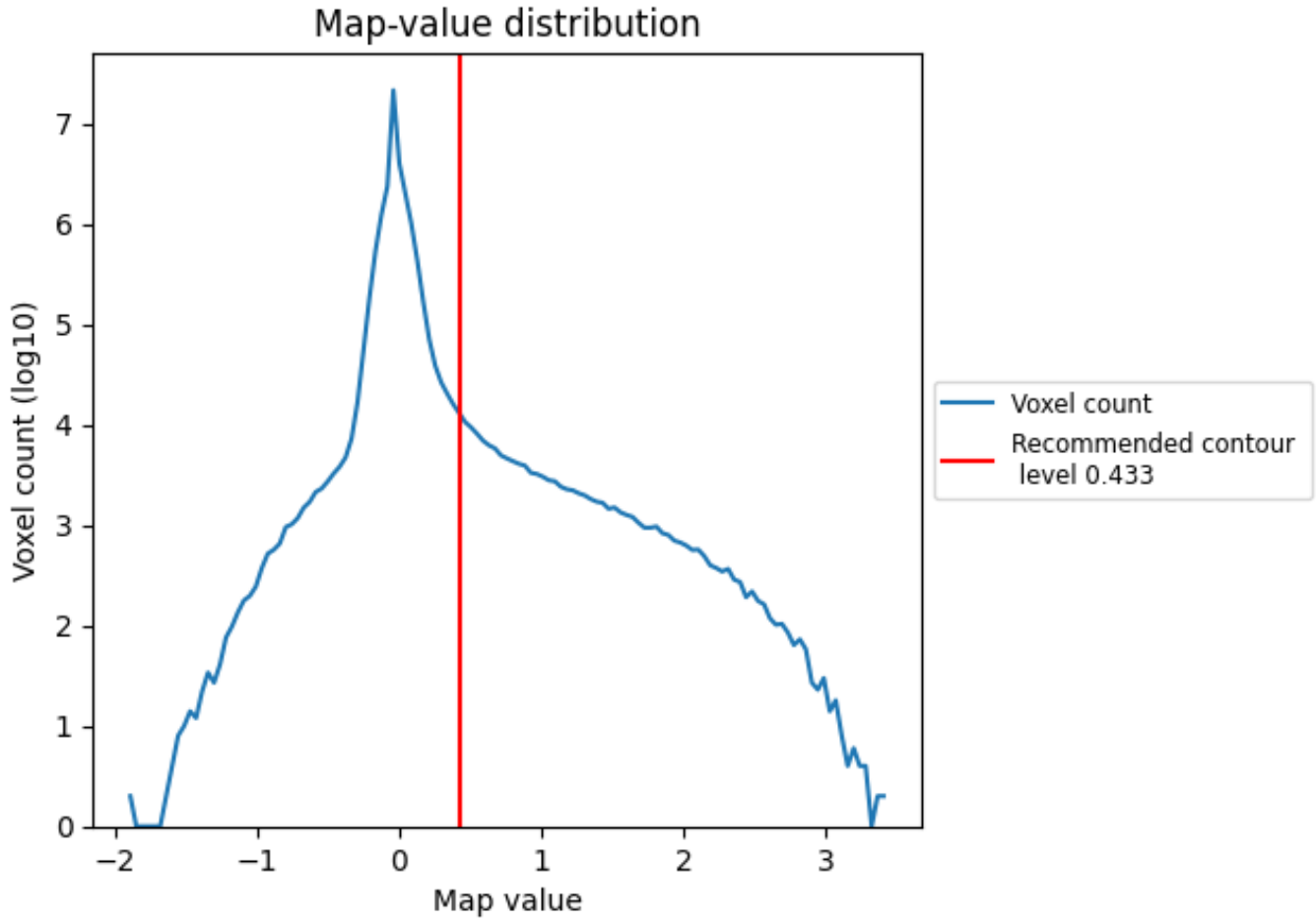
6.5 Mask visualisation (i)

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

7 Map analysis

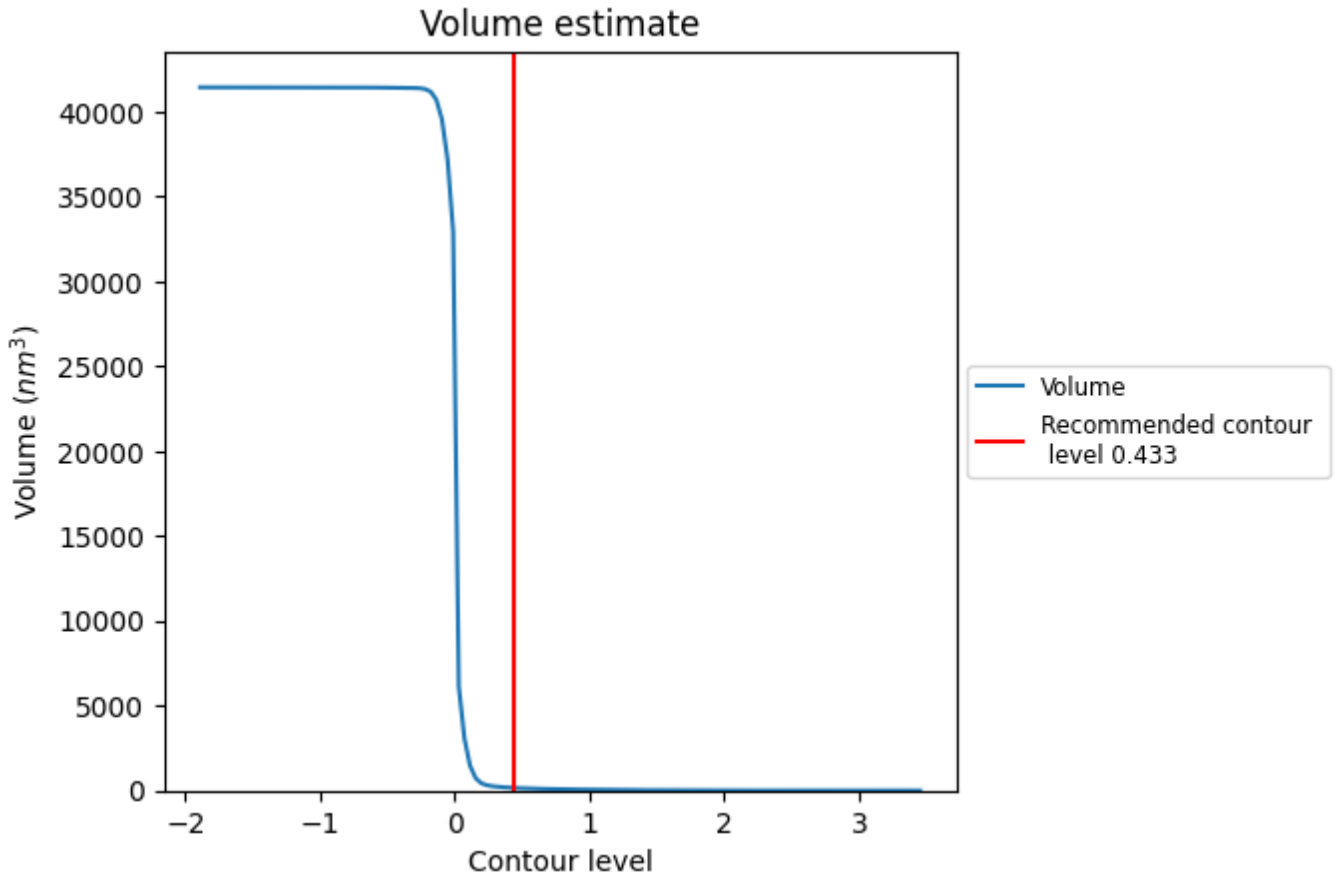
This section contains the results of statistical analysis of the map.

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.

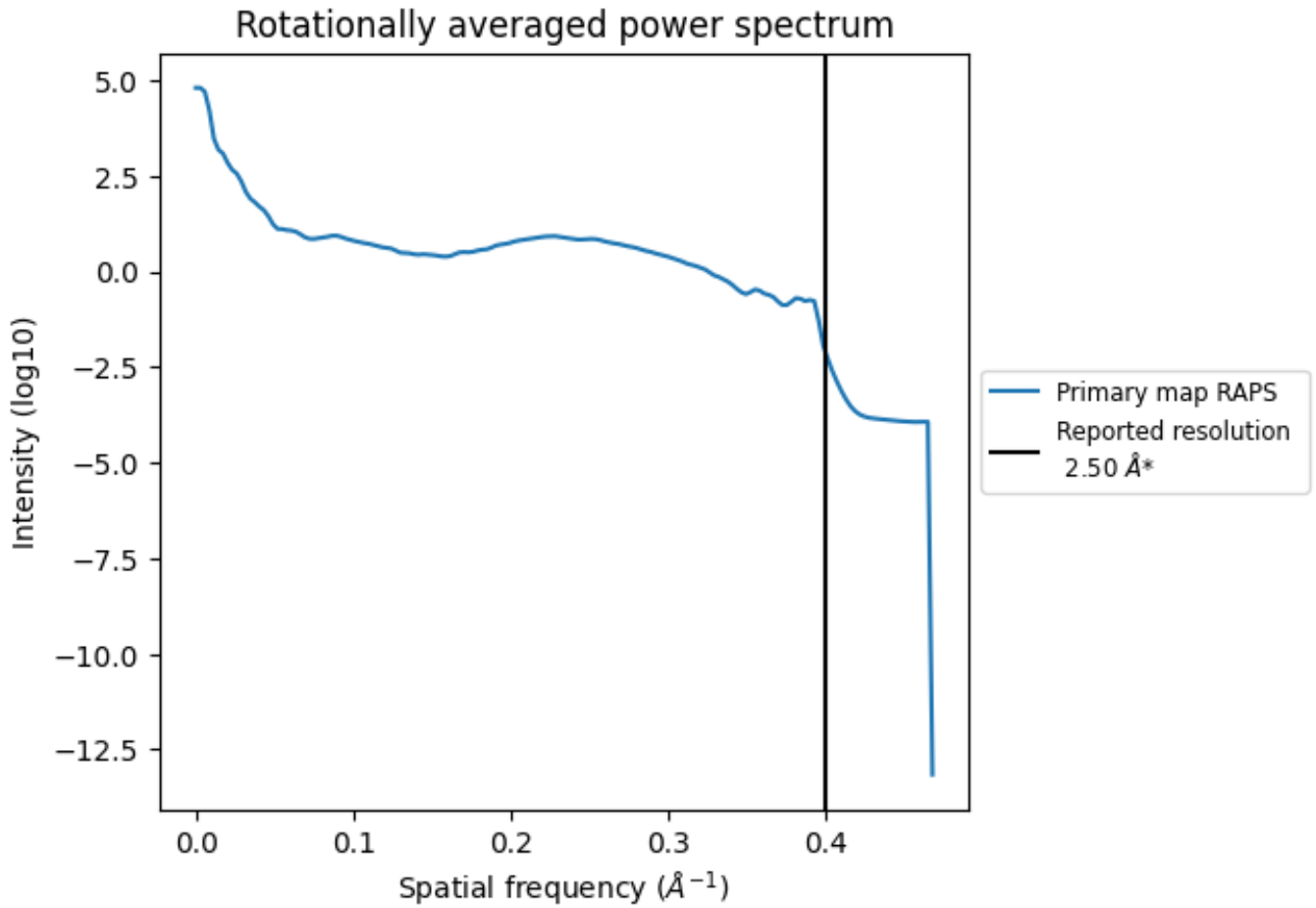
7.2 Volume estimate



The volume at the recommended contour level is 159 nm^3; this corresponds to an approximate mass of 144 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 0.400 Å^{-1}

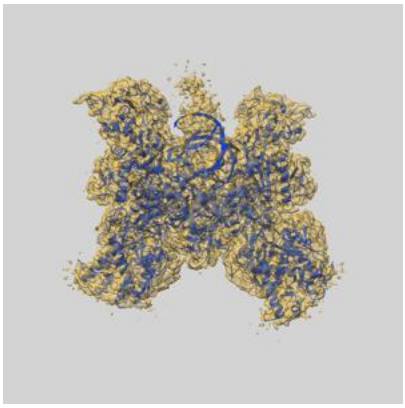
8 Fourier-Shell correlation

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

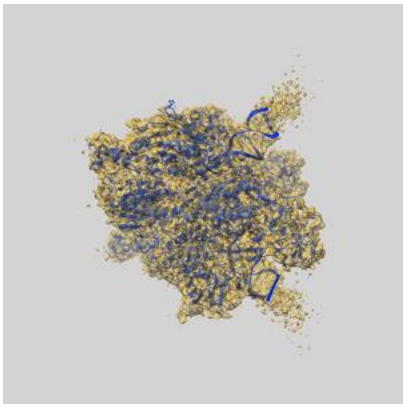
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24104 and PDB model 7N0D. Per-residue inclusion information can be found in section 3 on page 7.

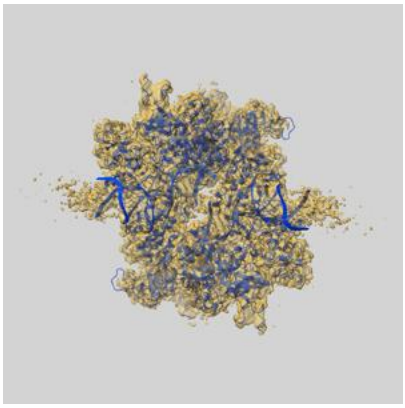
9.1 Map-model overlay



X



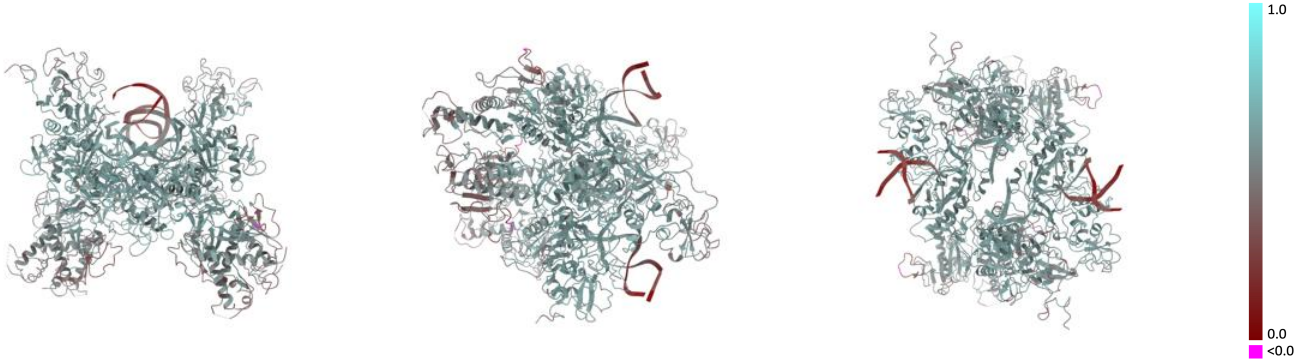
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.433 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

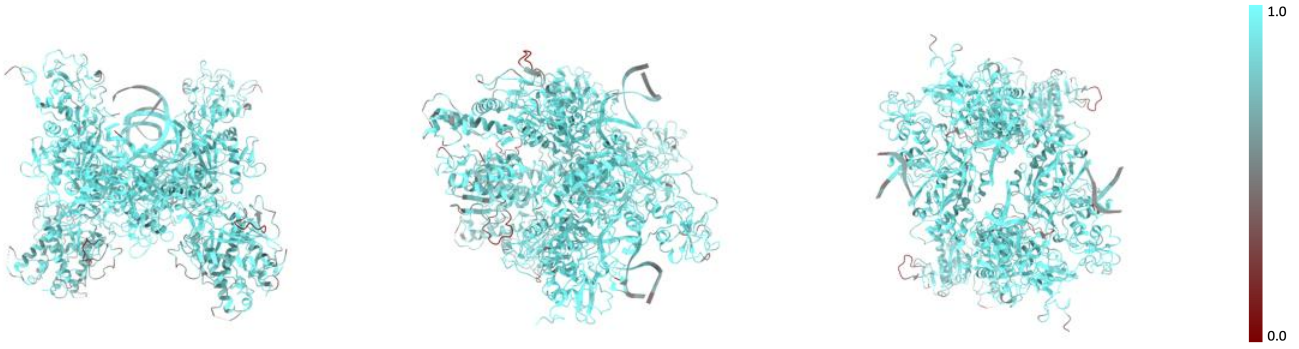
9.2 Q-score mapped to coordinate model



X Y Z

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

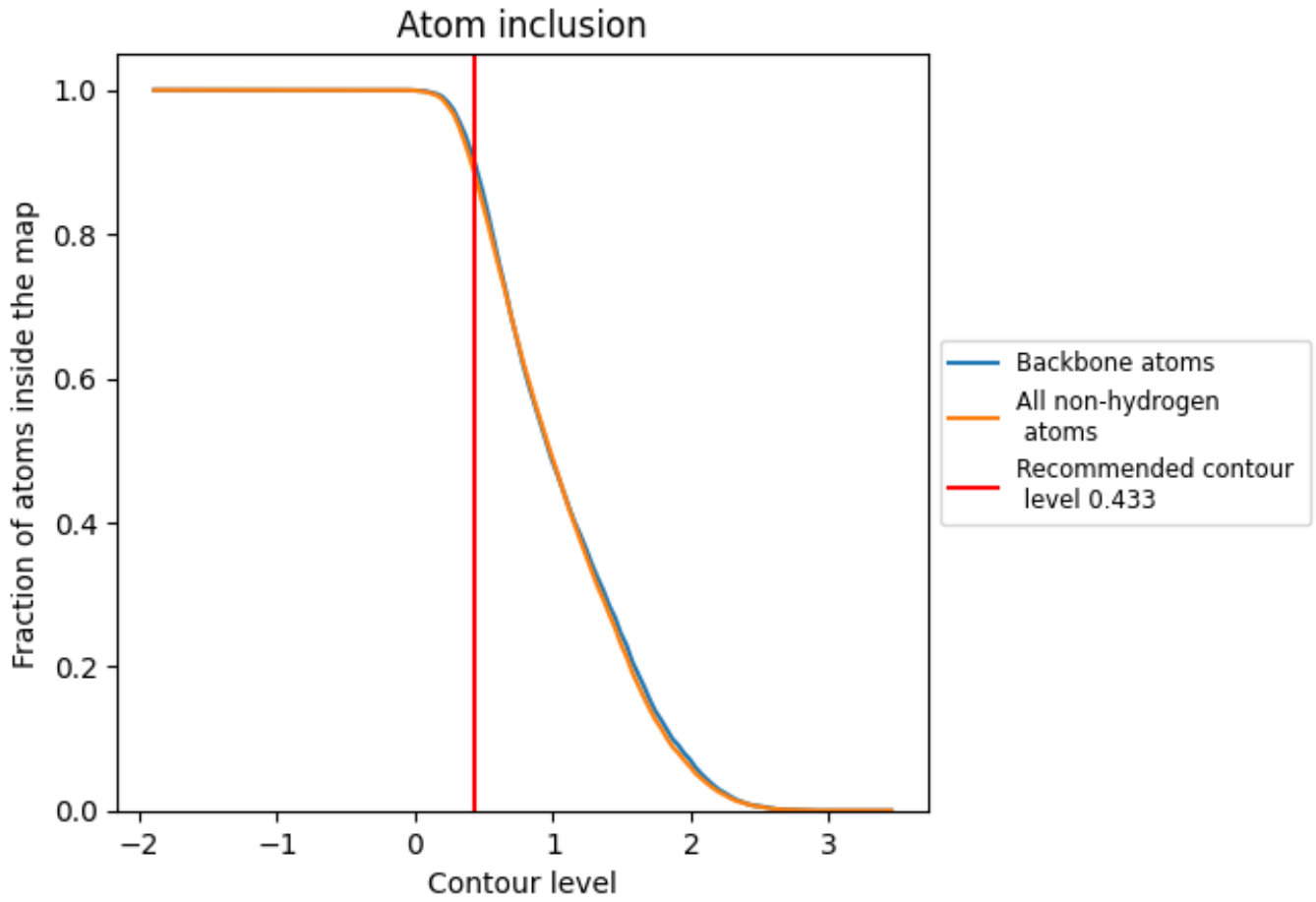
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.433).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.433) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8840	0.5420
A	0.9389	0.5800
B	0.8904	0.5570
C	0.8904	0.5380
D	0.8764	0.5380
E	0.9399	0.5800
F	0.8916	0.5560
G	0.8872	0.5410
H	0.8764	0.5390
I	0.8248	0.4410
J	0.9900	0.5970
K	0.8562	0.4010
L	0.8459	0.3980
P	0.9900	0.5840
T	0.8321	0.4490