wwPDB EM Validation Summary Report (i)

Mar 20, 2024 – 01:43 PM JST

PDB ID	:	7D4F
EMDB ID	:	EMD-30572
Title	:	Structure of COVID-19 RNA-dependent RNA polymerase bound to suramin
Authors	:	Li, Z.; Yin, W.; Zhou, Z.; Yu, X.; Xu, H.
Deposited on	:	2020-09-23
Resolution	:	2.57 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 (1)) were used in the production of this report:

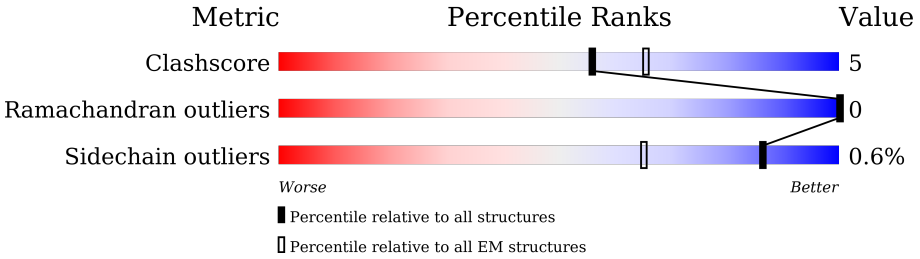
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.57 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	B	199	50% 7% 43%
1	G	199	22% 45% 9% 47%
2	C	84	61% 14% 25%
3	A	943	87% 8% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9534 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 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	114	882	557	148	170	7	0	0
1	G	106	820	518	135	160	7	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P0DTD1
G	0	MET	-	initiating methionine	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	63	485	307	80	93	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P0DTD1

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	898	7261	4648	1220	1342	51	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0DTD1

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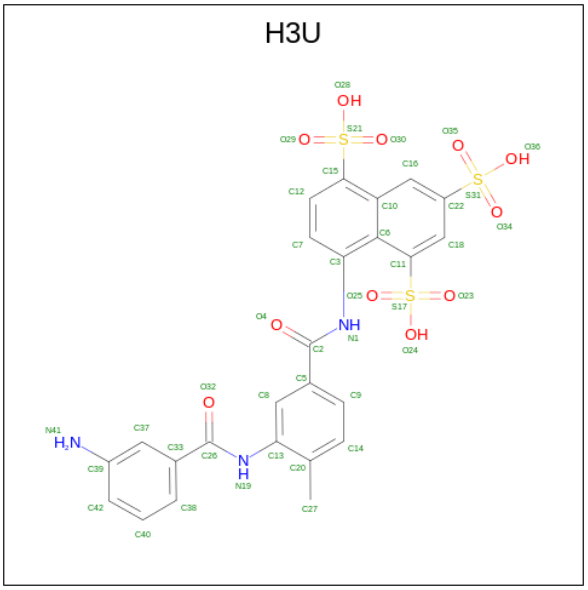
Chain	Residue	Modelled	Actual	Comment	Reference
A	933	GLY	-	expression tag	UNP P0DTD1
A	934	GLY	-	expression tag	UNP P0DTD1
A	935	SER	-	expression tag	UNP P0DTD1
A	936	GLU	-	expression tag	UNP P0DTD1
A	937	ASN	-	expression tag	UNP P0DTD1
A	938	LEU	-	expression tag	UNP P0DTD1
A	939	TYR	-	expression tag	UNP P0DTD1
A	940	PHE	-	expression tag	UNP P0DTD1
A	941	GLN	-	expression tag	UNP P0DTD1
A	942	GLY	-	expression tag	UNP P0DTD1

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
4	A	2	2	2	0

- Molecule 5 is 8-(3-(3-aminobenzamido)-4-methylbenzamido)naphthalene-1,3,5-trisulfonic acid (three-letter code: H3U) (formula: $C_{25}H_{21}N_3O_{11}S_3$) (labeled as "Ligand of Interest" by depositor).

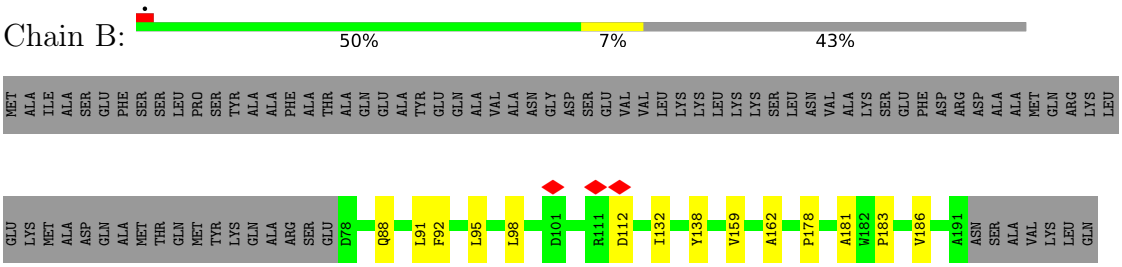


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	42	25	3	11	3	0
			Total	C	N	O	S	
5	A	1	42	25	3	11	3	0

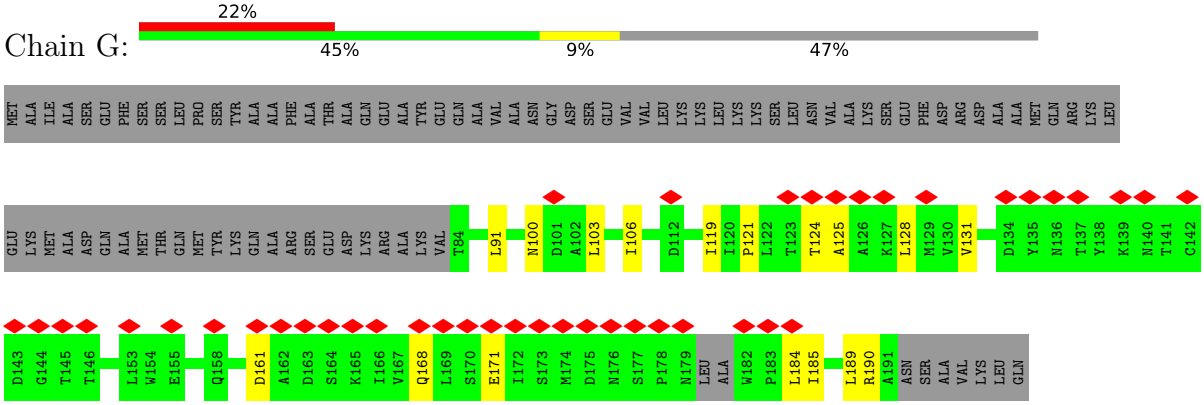
3 Residue-property plots (i)

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.

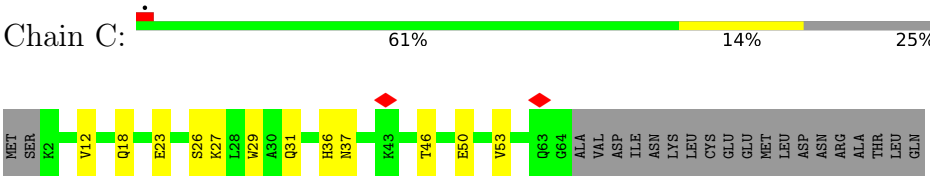
• Molecule 1: Non-structural protein 8



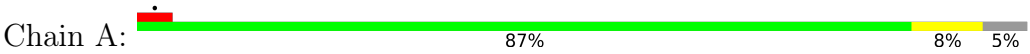
• Molecule 1: Non-structural protein 8

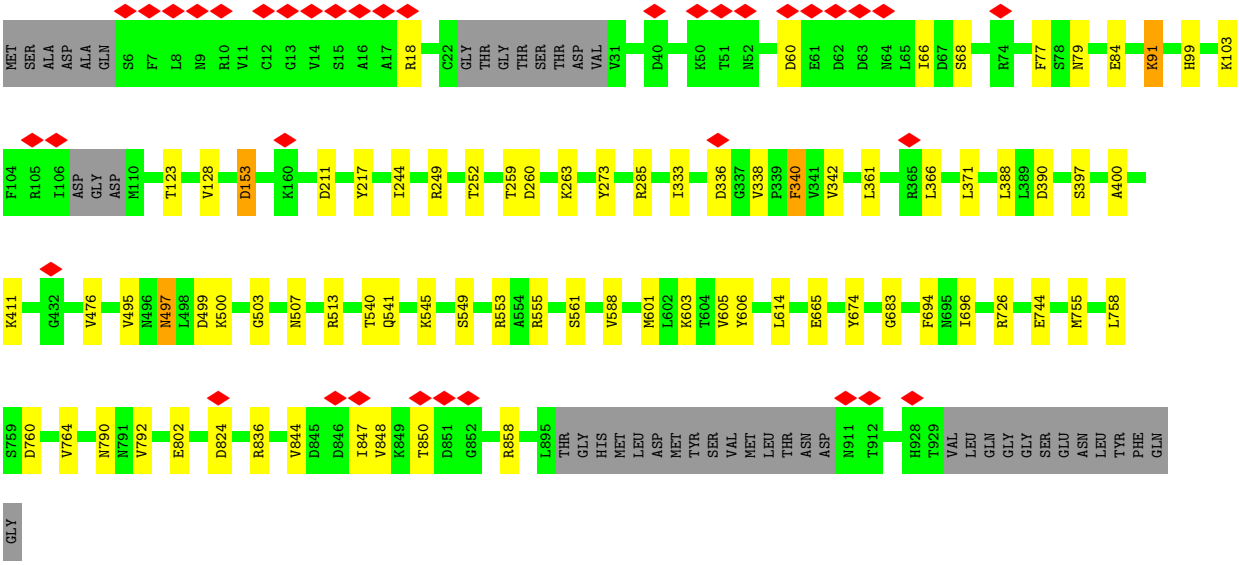


• Molecule 2: Non-structural protein 7



• Molecule 3: RNA-directed RNA polymerase




MET SER ALA ASP ALA GLN S6 F7 L8 N9 R10 V11 C12 G13 V14 S15 A16 A17 R18 C22 GLY THR GLY THR SER THR ASP VAL V31 D40 K50 T51 N52 D60 E61 D62 D63 N64 L65 I66 D67 S68 R74 F77 S78 N79 E84 K91 H99 K103
F104 R105 I106 ASP GLY ASP M110 T123 V128 D153 K160 D211 Y217 I244 R249 T252 T259 D260 K263 Y273 R285 I333 D336 G337 V338 P339 F340 V341 V342 L361 R365 L366 L371 L388 L389 D390 S397 A400
K411 G432 V476 V495 N496 N497 L498 D499 K500 G503 N507 R513 T540 Q541 K545 S549 R553 A554 R555 S561 V588 M601 L602 K603 T604 V605 Y606 L614 E665 Y674 G683 F694 N695 I696 R726 E744 M755 L758
S759 D760 V764 N790 N791 V792 E802 D824 R836 V844 D845 D846 I847 V848 K849 T850 D851 G852 R858 L895 THR GLY HIS MET LEU ASP MET TYR SER VAL MET LEU THR ASN ASP N911 T912 H928 T929 VAL LEU GLN GLY GLY SER GLU ASN LEU TYR PHE GLN
GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	95845	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 ($e^-/Å^2$)	68	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	0.205	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	273.664, 273.664, 273.664	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.069, 1.069, 1.069	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: H3U, ZN

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	B	0.42	0/895	0.56	0/1221
1	G	0.38	0/832	0.60	0/1136
2	C	0.43	0/488	0.54	0/657
3	A	0.47	0/7445	0.54	3/10098 (0.0%)
All	All	0.46	0/9660	0.55	3/13112 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	760	ASP	CB-CG-OD1	9.51	126.86	118.30
3	A	336	ASP	CB-CG-OD1	5.43	123.19	118.30
3	A	824	ASP	CB-CG-OD2	5.21	122.99	118.30

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	B	882	0	900	19	0
1	G	820	0	826	13	0
2	C	485	0	515	12	0
3	A	7261	0	7020	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
5	A	84	0	0	13	0
All	All	9534	0	9261	98	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 5.

The worst 5 of 98 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:B:95:LEU:HD11	3:A:338:VAL:CG1	1.83	1.08
3:A:497:ASN:HD22	3:A:497:ASN:H	1.22	0.87
5:A:1003:H3U:N1	5:A:1003:H3U:O25	2.08	0.87
1:B:95:LEU:HD11	3:A:338:VAL:HG12	1.57	0.86
3:A:553:ARG:NH1	5:A:1004:H3U:O34	2.09	0.85

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	B	112/199 (56%)	109 (97%)	3 (3%)	0	100	100
1	G	102/199 (51%)	100 (98%)	2 (2%)	0	100	100
2	C	61/84 (73%)	61 (100%)	0	0	100	100
3	A	890/943 (94%)	869 (98%)	21 (2%)	0	100	100
All	All	1165/1425 (82%)	1139 (98%)	26 (2%)	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	B	100/168 (60%)	100 (100%)	0	100	100
1	G	94/168 (56%)	94 (100%)	0	100	100
2	C	59/78 (76%)	59 (100%)	0	100	100
3	A	795/831 (96%)	789 (99%)	6 (1%)	81	92
All	All	1048/1245 (84%)	1042 (99%)	6 (1%)	86	94

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	340	PHE
3	A	495	VAL
3	A	497	ASN
3	A	91	LYS
3	A	84	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	497	ASN
3	A	790	ASN
3	A	822	GLN
3	A	791	ASN
1	G	88	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
5	H3U	A	1003	-	43,45,45	2.72	22 (51%)	62,70,70	1.19	8 (12%)
5	H3U	A	1004	-	43,45,45	2.71	23 (53%)	62,70,70	1.36	7 (11%)

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	H3U	A	1003	-	-	4/34/34/34	0/4/4/4
5	H3U	A	1004	-	-	8/34/34/34	0/4/4/4

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1004	H3U	C26-N19	4.83	1.48	1.35
5	A	1003	H3U	O34-S31	4.63	1.67	1.43
5	A	1003	H3U	O29-S21	4.63	1.66	1.43
5	A	1004	H3U	C2-N1	4.60	1.48	1.35
5	A	1004	H3U	O30-S21	4.53	1.66	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1004	H3U	C3-N1-C2	-5.07	113.61	128.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1004	H3U	C11-C6-C10	3.86	119.97	116.34
5	A	1003	H3U	C20-C13-N19	3.67	124.52	118.81
5	A	1004	H3U	C5-C2-N1	3.12	122.78	115.92
5	A	1004	H3U	C20-C13-N19	2.60	122.86	118.81

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1004	H3U	C10-C15-S21-O28
5	A	1004	H3U	C10-C15-S21-O29
5	A	1004	H3U	C10-C15-S21-O30
5	A	1004	H3U	C12-C15-S21-O30
5	A	1003	H3U	C20-C13-N19-C26

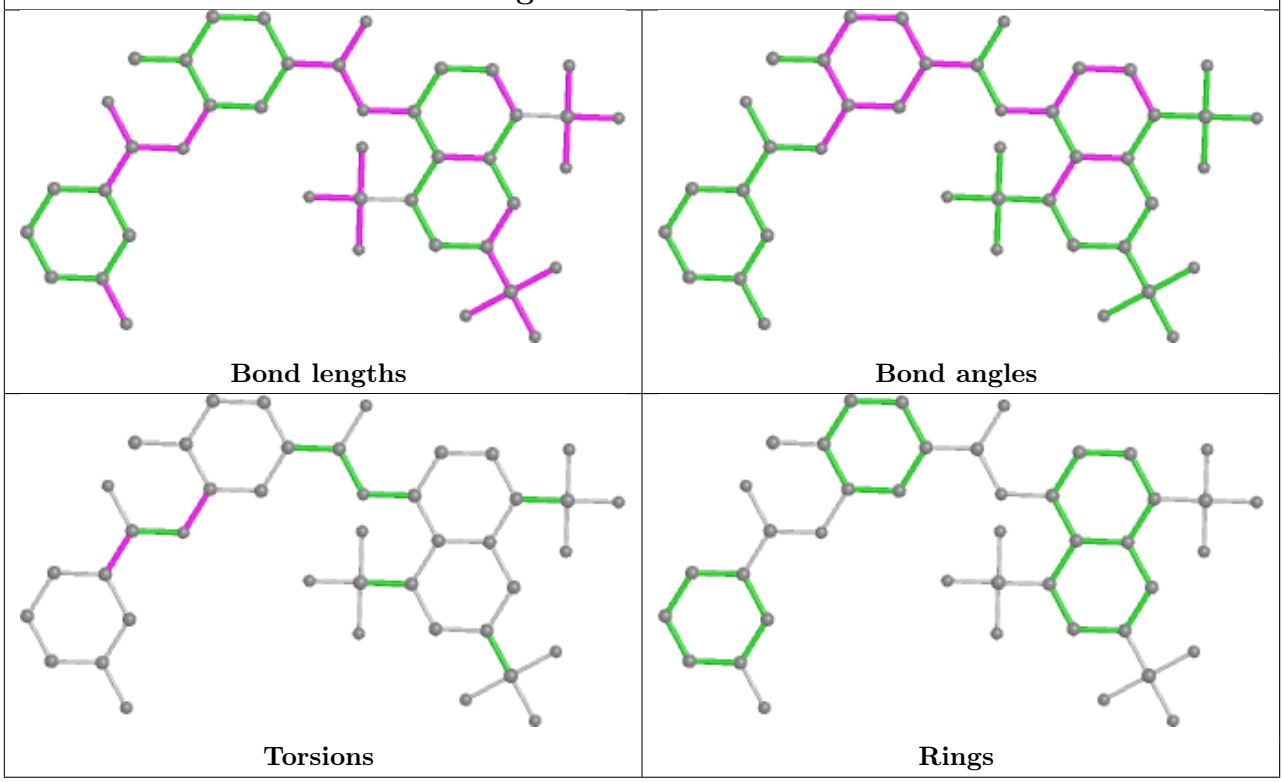
There are no ring outliers.

2 monomers are involved in 13 short contacts:

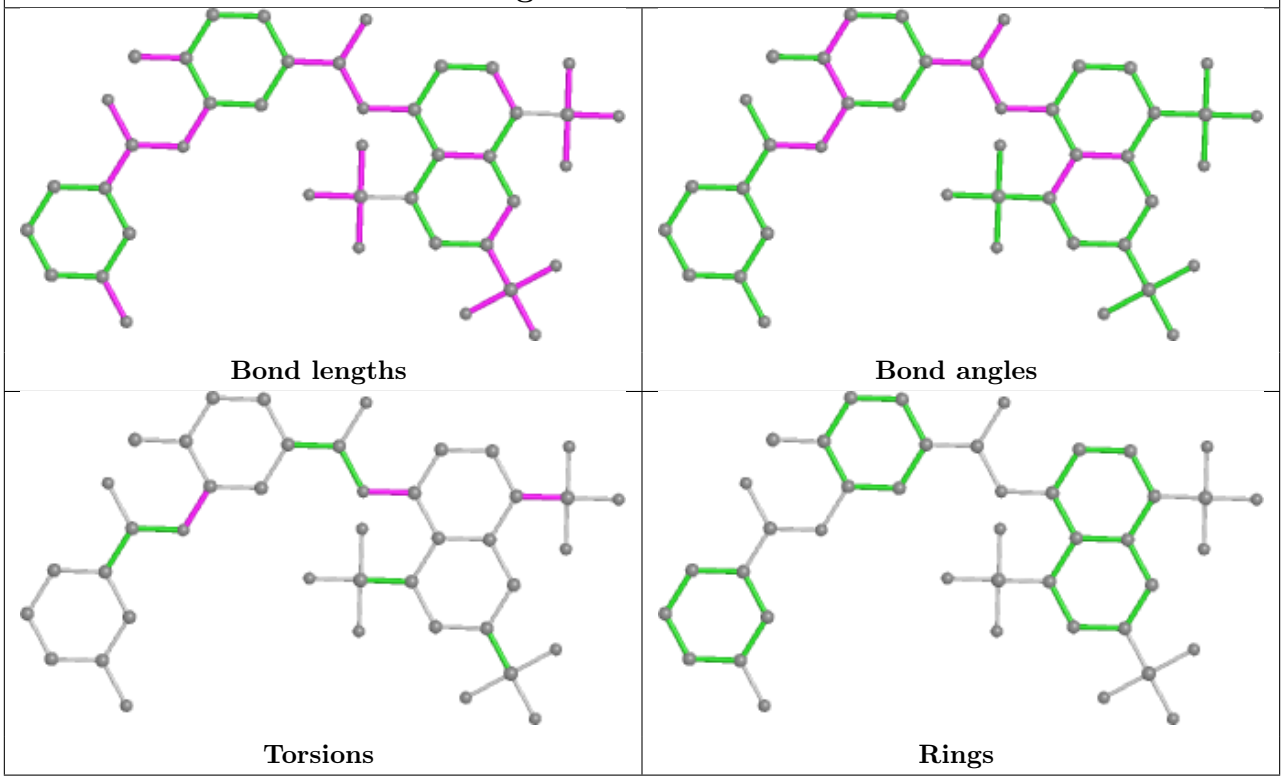
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1003	H3U	3	0
5	A	1004	H3U	10	0

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 H3U A 1003



Ligand H3U A 1004



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.

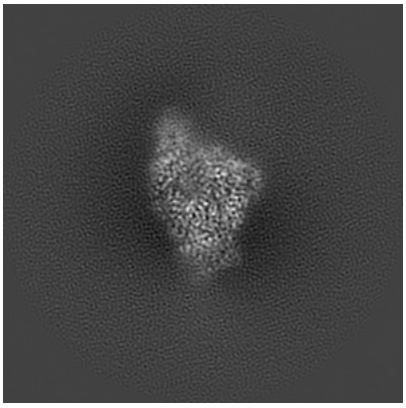
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30572. These allow visual inspection of the internal detail of the map and identification of artifacts.

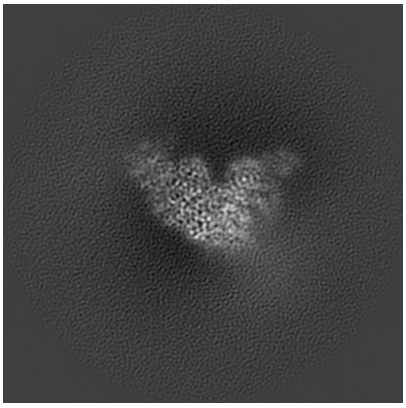
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

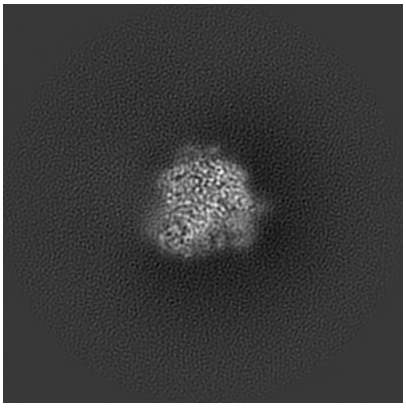
6.1.1 Primary map



X



Y

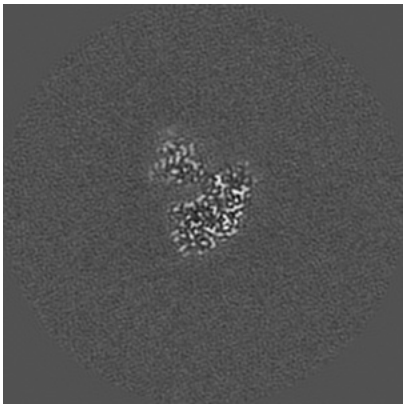


Z

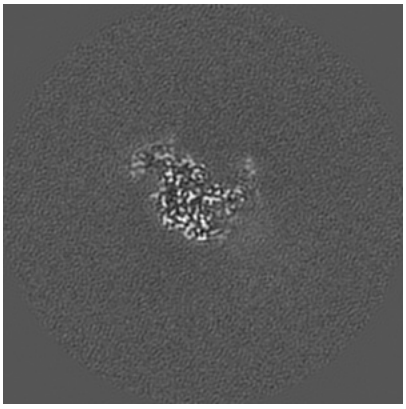
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

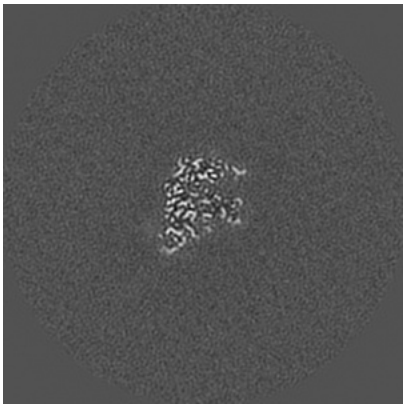
6.2.1 Primary map



X Index: 128



Y Index: 128

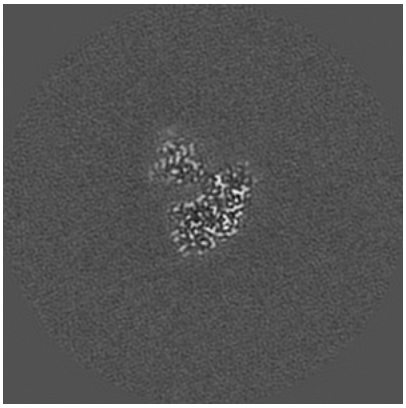


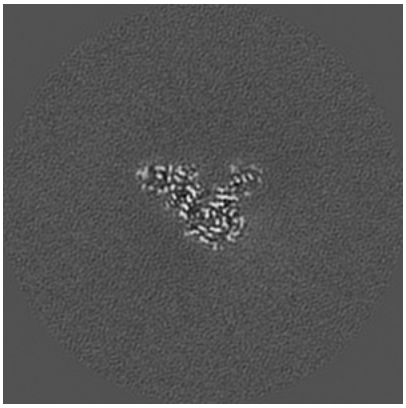
Z Index: 128

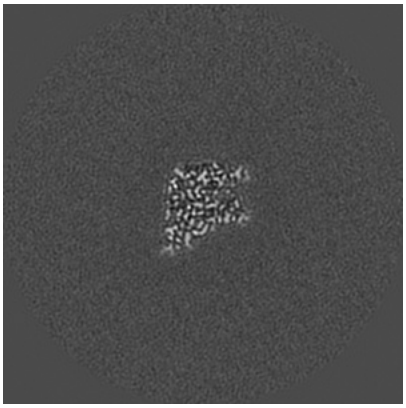
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 128

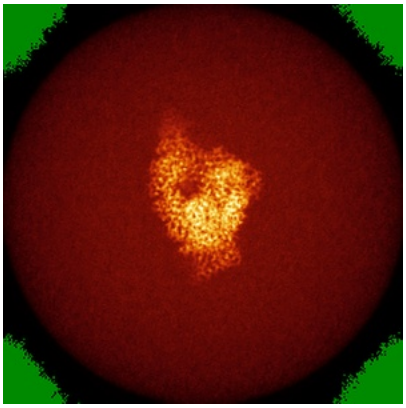

Y Index: 140

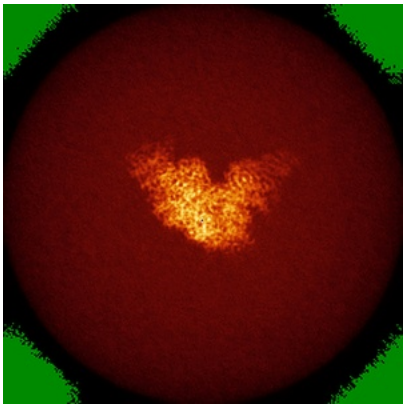

Z Index: 124

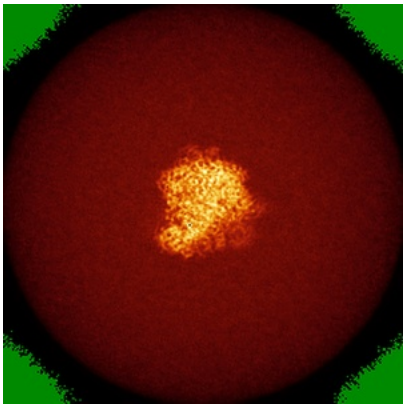
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

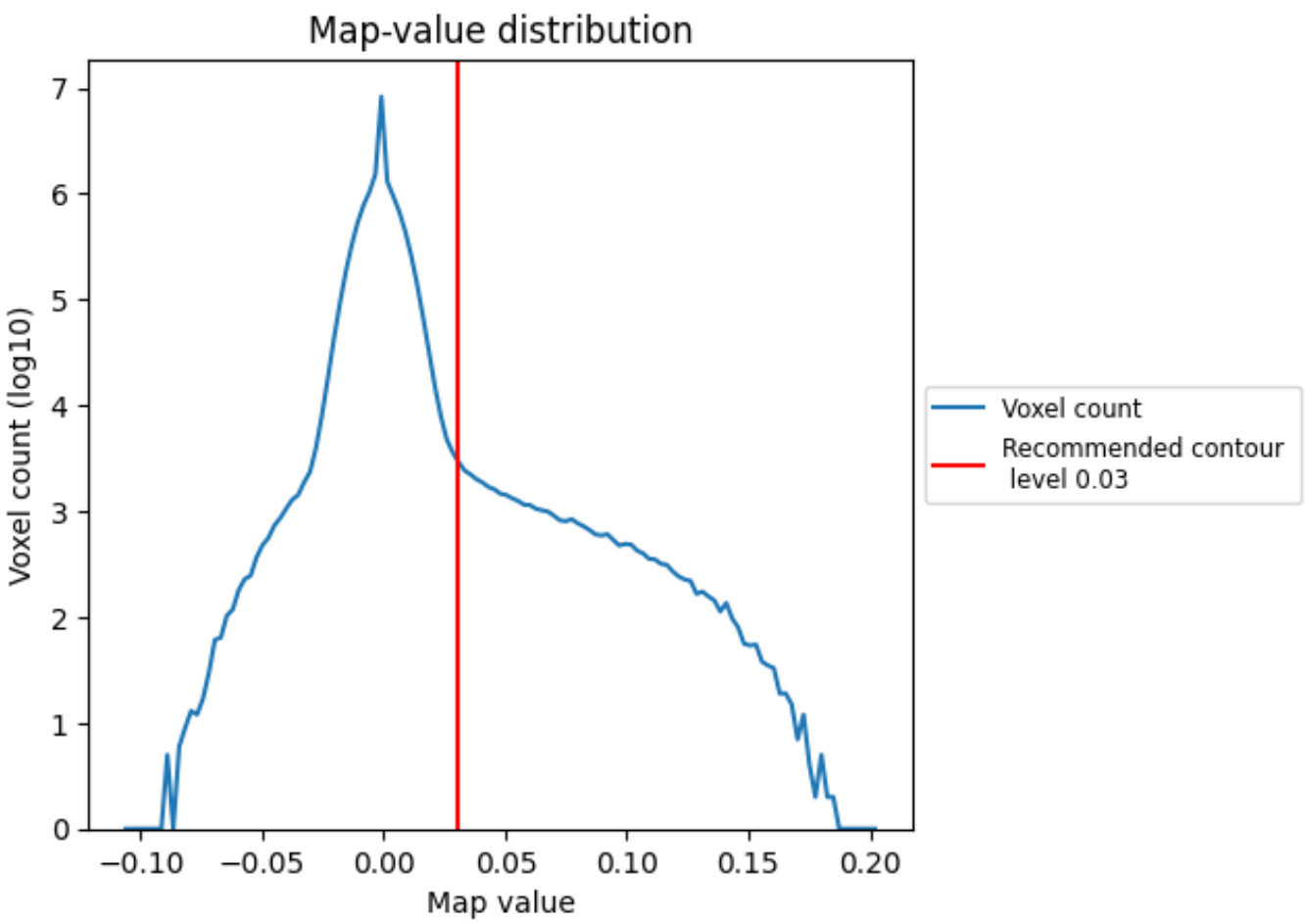
6.6 Mask visualisation (i)

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

7 Map analysis (i)

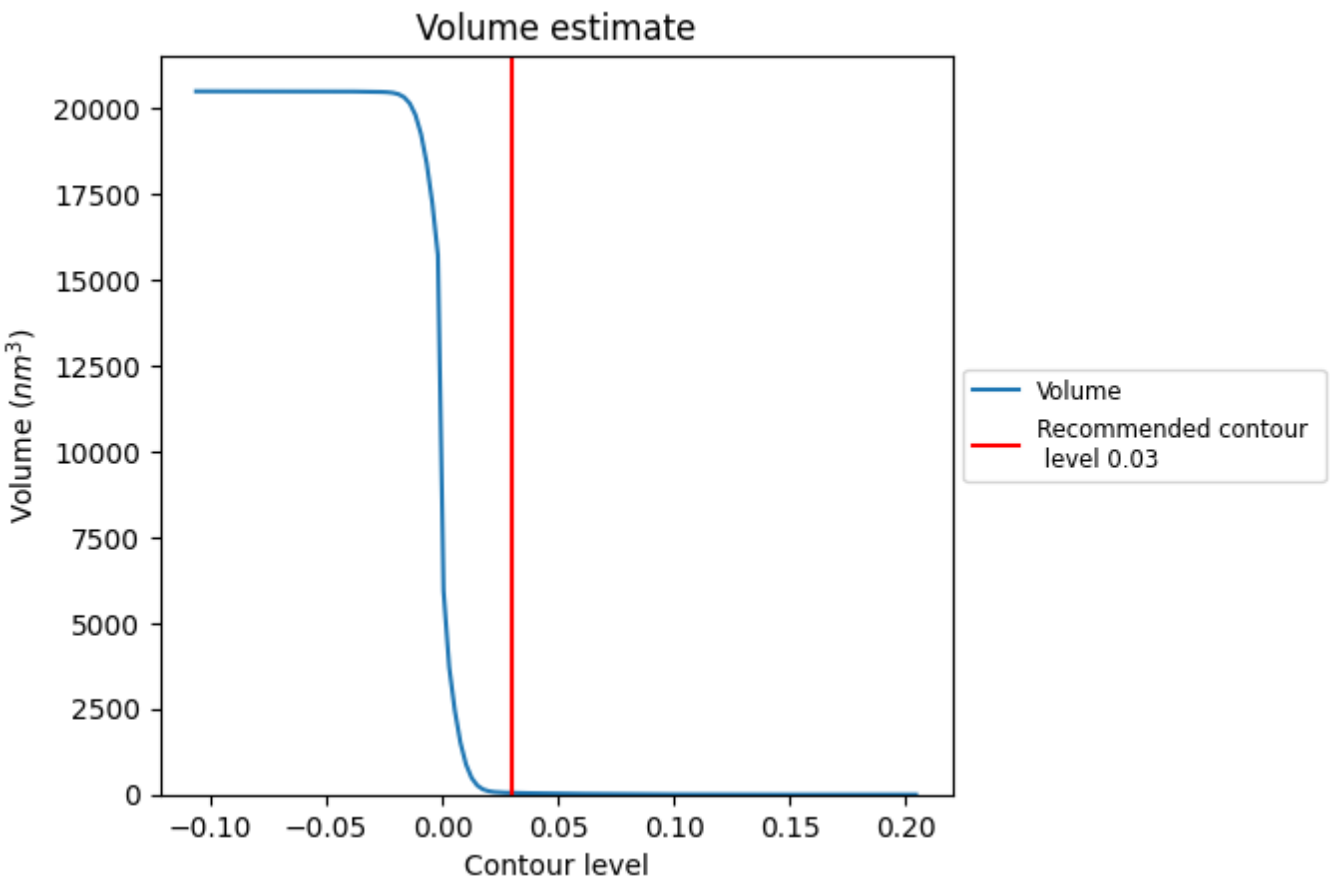
This section contains the results of statistical analysis of the map.

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.

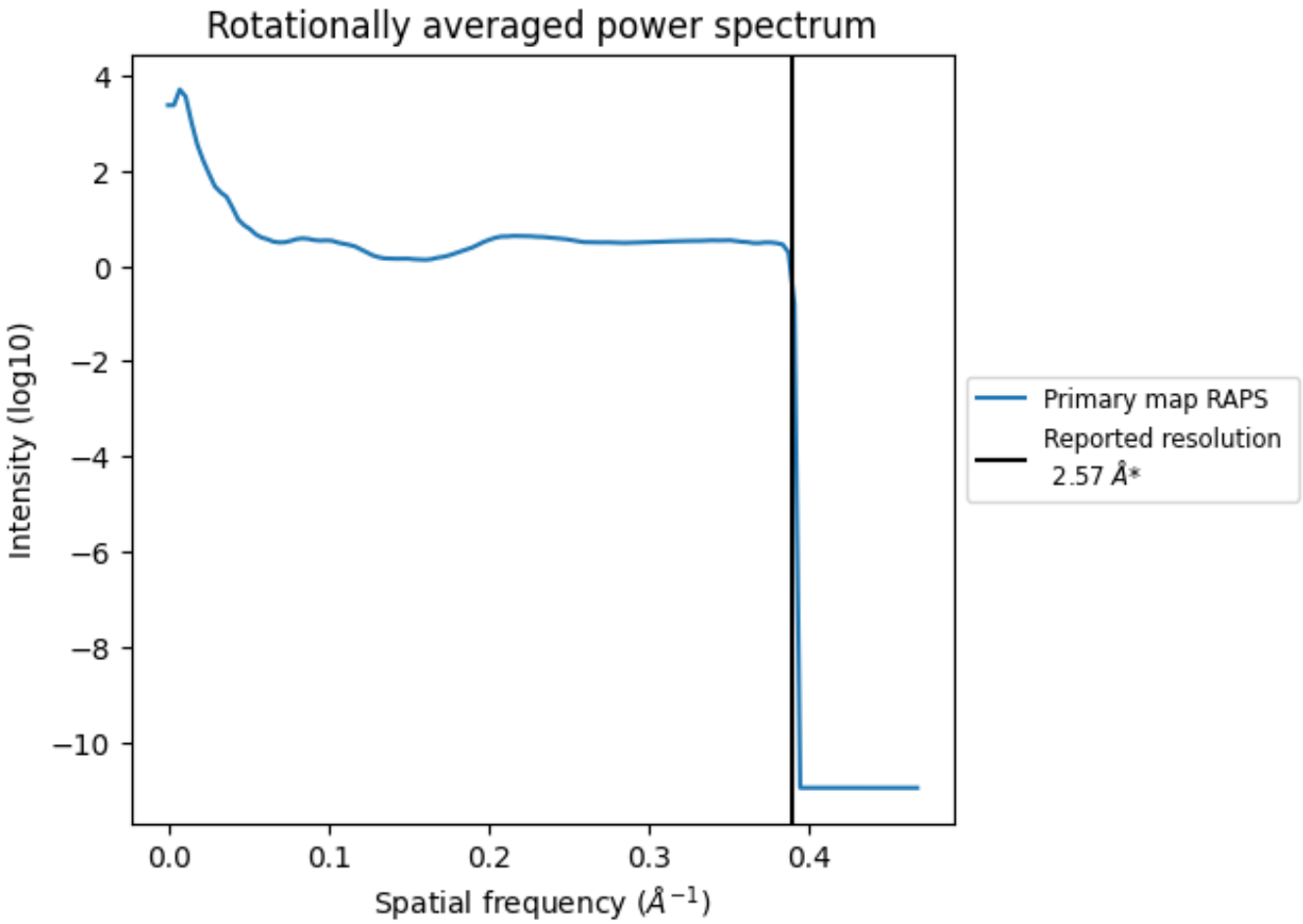
7.2 Volume estimate (i)



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 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 0.389 Å^{-1}

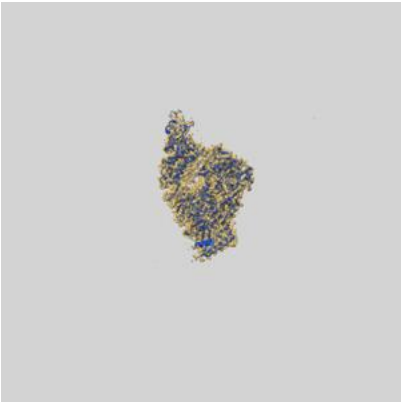
8 Fourier-Shell correlation (i)

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

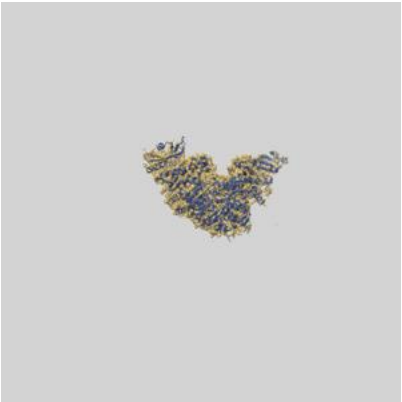
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30572 and PDB model 7D4F. Per-residue inclusion information can be found in section 3 on page 5.

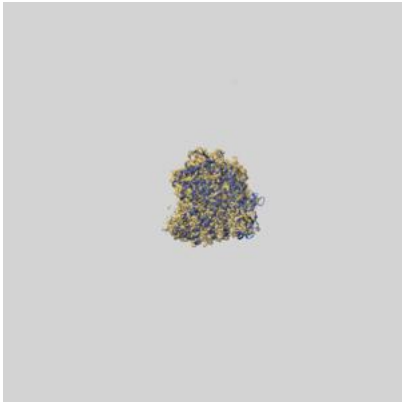
9.1 Map-model overlay (i)



X



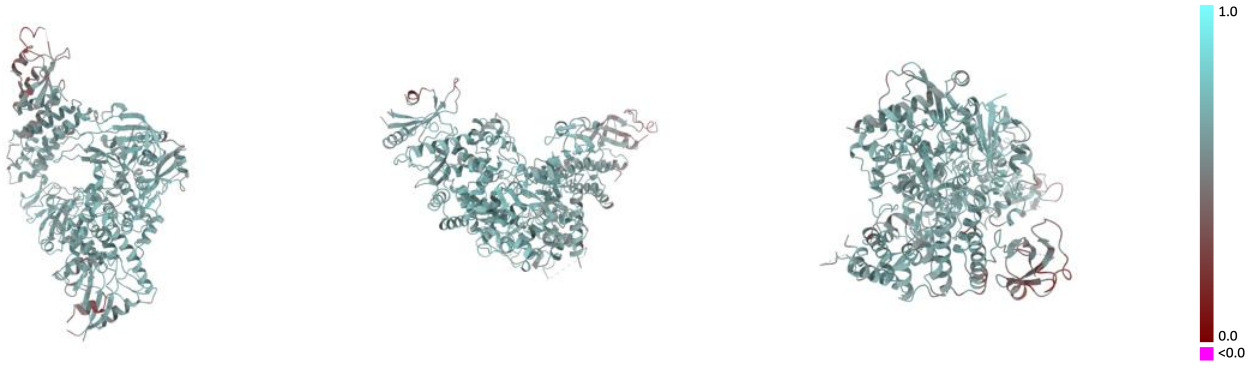
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

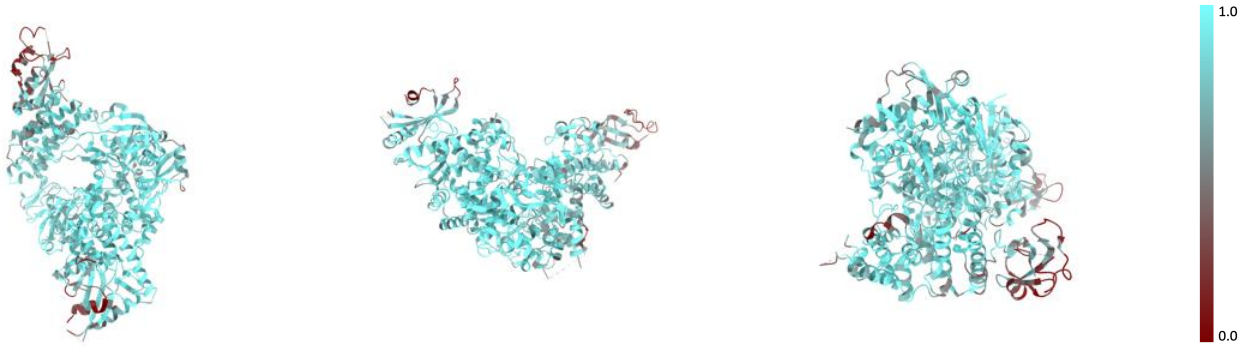
9.2 Q-score mapped to coordinate model (i)



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.

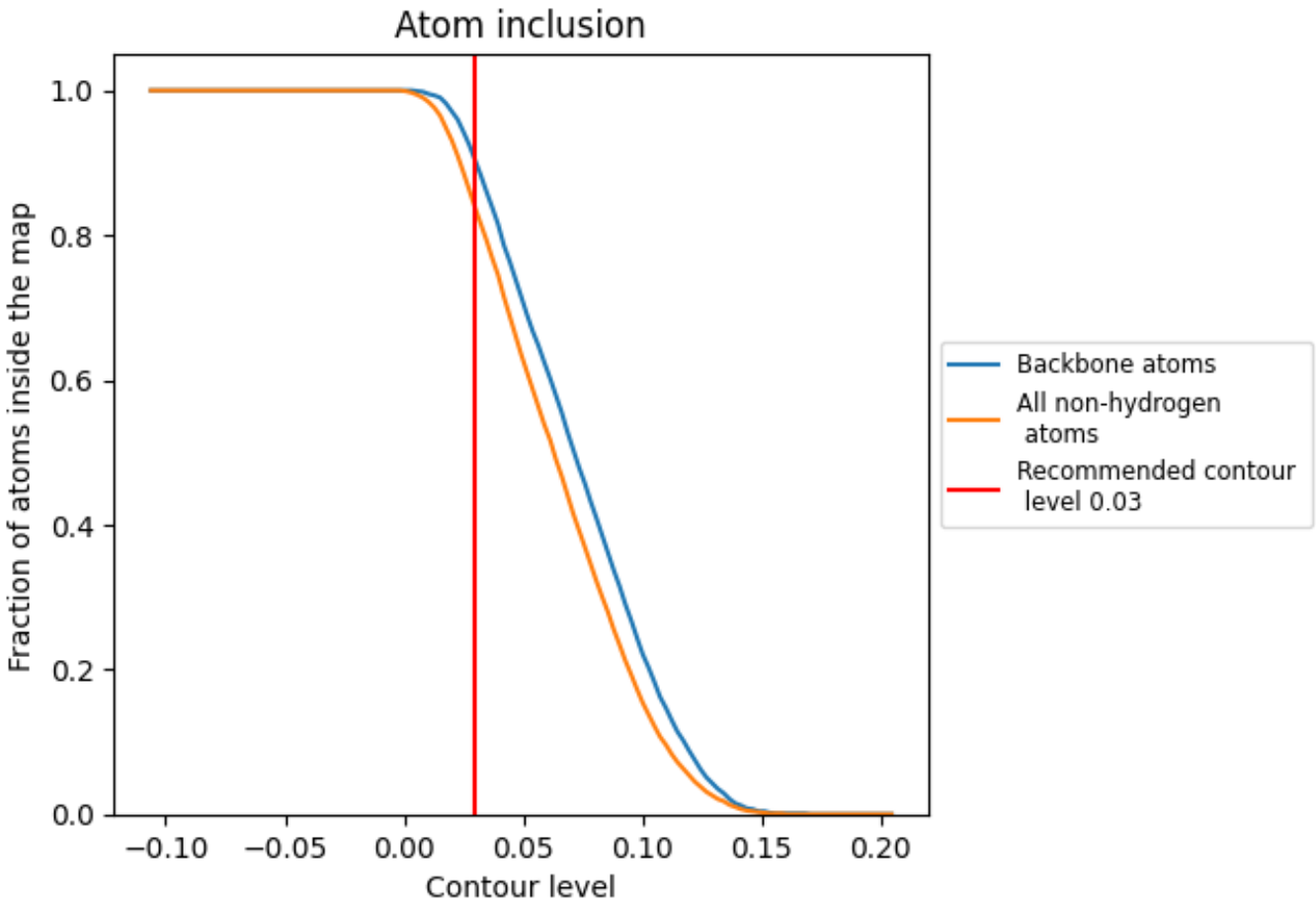
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.6080
A	0.8780	0.6260
B	0.8070	0.5960
C	0.8260	0.5950
G	0.4980	0.4660