



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 02:19 AM JST

PDB ID : 7CYQ
EMDB ID : EMD-30504
Title : Cryo-EM structure of an extended SARS-CoV-2 replication and transcription complex reveals an intermediate state in cap synthesis
Authors : Yan, L.; Ge, J.; Zheng, L.; Zhang, Y.; Gao, Y.; Wang, T.; Wang, H.; Huang, Y.; Li, M.; Wang, Q.; Rao, Z.; Lou, Z.
Deposited on : 2020-09-04
Resolution : 2.83 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) : 2.31.3

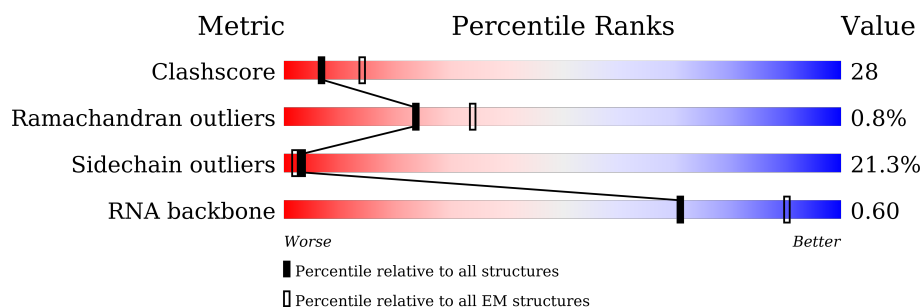
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	942	
2	B	198	
2	D	198	
3	C	83	
4	I	33	
5	J	59	
6	E	601	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	601	
7	G	117	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	GDP	A	1003	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21857 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 RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	926	7458	4763	1251	1390	54	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	933	HIS	-	expression tag	UNP P0DTD1
A	934	HIS	-	expression tag	UNP P0DTD1
A	935	HIS	-	expression tag	UNP P0DTD1
A	936	HIS	-	expression tag	UNP P0DTD1
A	937	HIS	-	expression tag	UNP P0DTD1
A	938	HIS	-	expression tag	UNP P0DTD1
A	939	HIS	-	expression tag	UNP P0DTD1
A	940	HIS	-	expression tag	UNP P0DTD1
A	941	HIS	-	expression tag	UNP P0DTD1
A	942	HIS	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	187	1396	872	240	273	11	0	0
2	D	186	1414	889	242	272	11	0	0

- Molecule 3 is a protein called Non-structural protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	72	553	349	91	107	6	0	0

- Molecule 4 is a RNA chain called Primer.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	25	Total	C	N	O	P	0	0
			545	242	105	173	25		

- Molecule 5 is a RNA chain called Template.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	27	Total	C	N	O	P	0	0
			565	253	94	191	27		

- Molecule 6 is a protein called Helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	585	Total	C	N	O	S	1	0
			4508	2875	750	848	35		
6	E	586	Total	C	N	O	S	1	0
			4513	2878	751	849	35		

- Molecule 7 is a protein called Non-structural protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	113	Total	C	N	O	S	0	0
			868	549	150	164	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	SER	-	expression tag	UNP P0DTD1
G	-2	ASN	-	expression tag	UNP P0DTD1
G	-1	ALA	-	expression tag	UNP P0DTD1
G	0	MET	-	expression tag	UNP P0DTD1

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

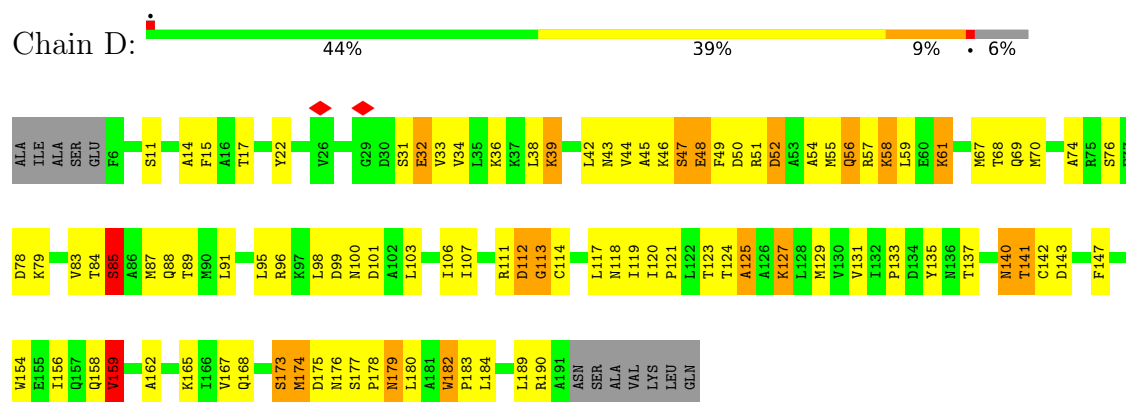
Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Zn	0
			2	2	
8	F	3	Total	Zn	0
			3	3	
8	E	3	Total	Zn	0
			3	3	

-
- The image displays the chemical structure of Guanosine Diphosphate (GDP). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system and amino group. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group having two hydroxyl groups. The structure is labeled with atom names and numbers, and the overall molecule is identified as GDP.

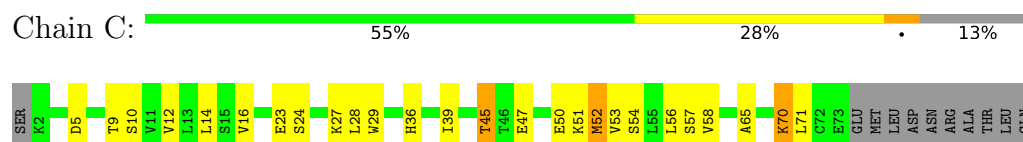
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mg 1 1	0

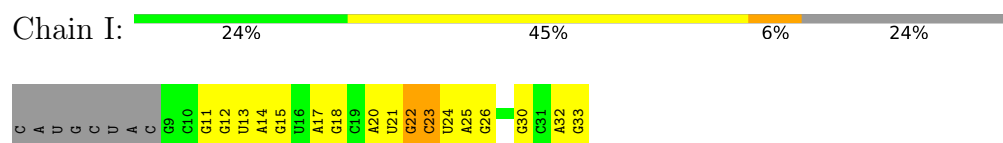
- Molecule 2: Non-structural protein 8



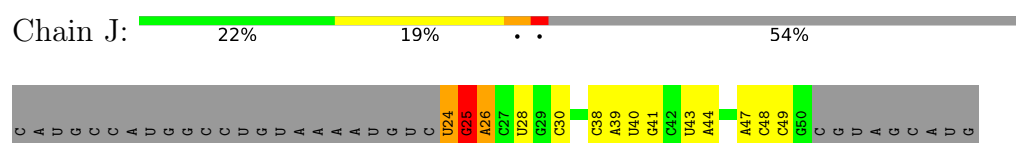
- Molecule 3: Non-structural protein 7



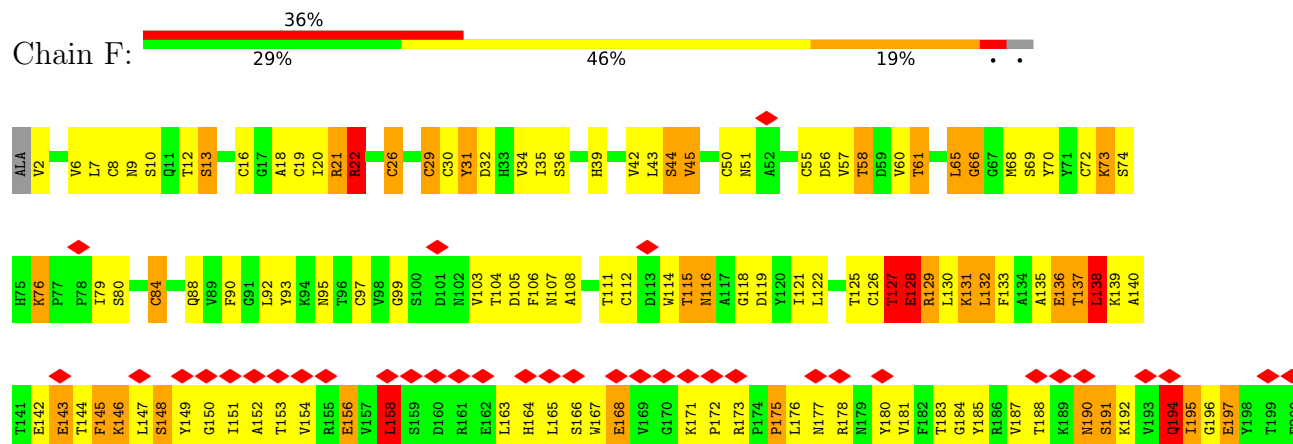
- Molecule 4: Primer

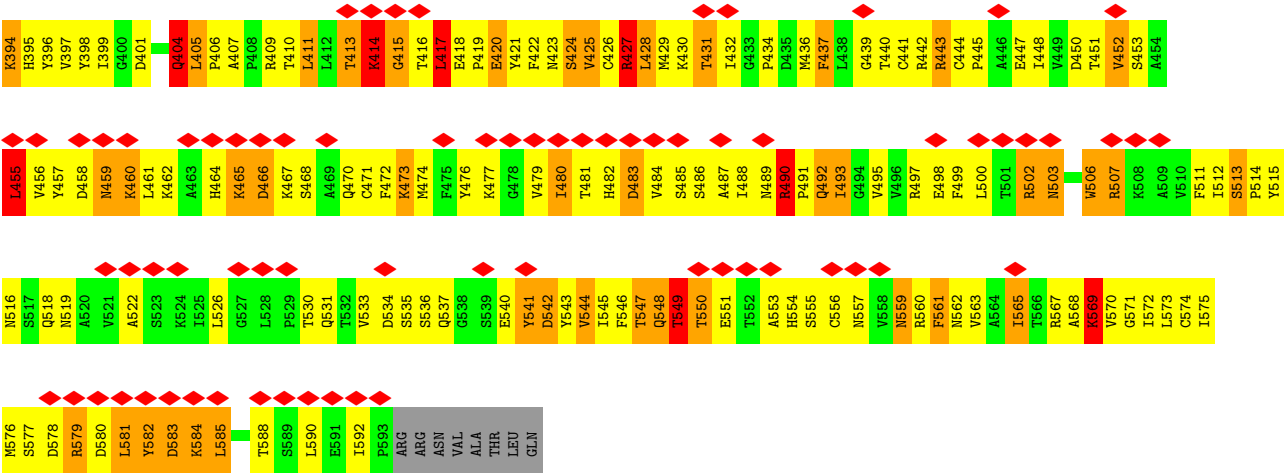


- Molecule 5: Template

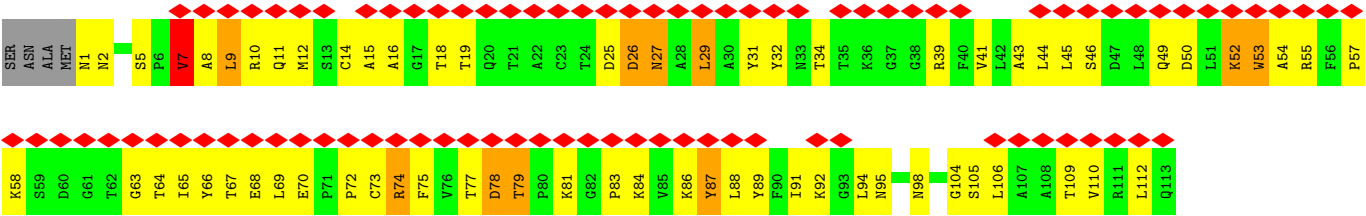
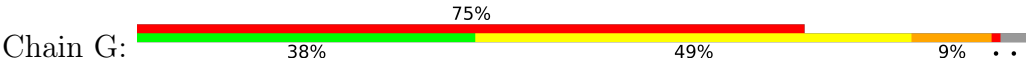


- Molecule 6: Helicase





● Molecule 7: Non-structural protein 9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	529558	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.146	Depositor
Minimum map value	-0.897	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.25	Depositor
Map size (\AA)	367.36, 367.36, 367.36	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, 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	A	0.73	1/7647 (0.0%)	0.75	32/10379 (0.3%)
2	B	0.60	0/1414	0.83	6/1922 (0.3%)
2	D	0.41	0/1433	0.73	6/1944 (0.3%)
3	C	0.54	0/556	0.56	0/749
4	I	0.89	1/611 (0.2%)	0.88	0/953
5	J	1.07	3/628 (0.5%)	0.84	0/974
6	E	0.37	1/4615 (0.0%)	1.00	41/6290 (0.7%)
6	F	0.37	1/4610 (0.0%)	0.88	32/6283 (0.5%)
7	G	0.36	0/884	0.77	4/1200 (0.3%)
All	All	0.58	7/22398 (0.0%)	0.84	121/30694 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
2	D	0	1
6	E	0	1
6	F	0	2
7	G	0	1
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	26	A	O3'-P	-7.94	1.51	1.61
5	J	25	G	O3'-P	-7.63	1.51	1.61
5	J	24	U	O3'-P	-6.42	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	32	A	N9-C4	-6.26	1.34	1.37
6	E	26	CYS	CB-SG	-5.46	1.73	1.81

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ASN	CB-CA-C	-17.36	75.68	110.40
6	E	235	LEU	CB-CA-C	-16.05	79.70	110.20
6	E	405	LEU	N-CA-CB	-15.54	79.32	110.40
6	E	404	GLN	CB-CA-C	-15.53	79.33	110.40
1	A	855	MET	CB-CA-C	-15.27	79.87	110.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ASP	Peptide
1	A	903	TYR	Peptide
2	B	182	TRP	Peptide
2	D	38	LEU	Peptide
6	F	415	GLY	Peptide

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	A	7458	0	7191	174	0
2	B	1396	0	1364	75	0
2	D	1414	0	1416	80	0
3	C	553	0	585	21	0
4	I	545	0	272	23	0
5	J	565	0	291	27	0
6	E	4513	0	4431	370	0
6	F	4508	0	4423	378	0
7	G	868	0	880	61	0
8	A	2	0	0	0	0
8	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	3	0	0	0	0
9	A	28	0	12	10	0
10	A	1	0	0	0	0
All	All	21857	0	20865	1177	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 28.

The worst 5 of 1177 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:125:ALA:O	2:D:189:LEU:CD1	1.76	1.33
6:E:194:GLN:O	6:E:194:GLN:CG	1.70	1.33
2:B:41:SER:O	2:B:44:VAL:HG23	1.30	1.30
2:B:42:LEU:O	2:B:45:ALA:HB3	1.39	1.22
6:E:549:THR:CG2	6:E:549:THR:O	1.87	1.21

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	924/942 (98%)	853 (92%)	67 (7%)	4 (0%)	34	56
2	B	185/198 (93%)	163 (88%)	19 (10%)	3 (2%)	9	21
2	D	184/198 (93%)	159 (86%)	24 (13%)	1 (0%)	29	51
3	C	70/83 (84%)	69 (99%)	1 (1%)	0	100	100
6	E	581/601 (97%)	485 (84%)	91 (16%)	5 (1%)	17	34
6	F	580/601 (96%)	486 (84%)	87 (15%)	7 (1%)	13	28
7	G	111/117 (95%)	96 (86%)	13 (12%)	2 (2%)	8	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2635/2740 (96%)	2311 (88%)	302 (12%)	22 (1%)	24	38

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	847	ILE
2	B	183	PRO
2	B	57	ARG
2	B	98	LEU
6	F	352	LEU

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	817/833 (98%)	749 (92%)	68 (8%)	11	24
2	B	144/167 (86%)	123 (85%)	21 (15%)	3	6
2	D	149/167 (89%)	116 (78%)	33 (22%)	1	0
3	C	67/77 (87%)	62 (92%)	5 (8%)	13	28
6	E	498/523 (95%)	327 (66%)	171 (34%)	0	0
6	F	498/523 (95%)	325 (65%)	173 (35%)	0	0
7	G	94/97 (97%)	83 (88%)	11 (12%)	5	10
All	All	2267/2387 (95%)	1785 (79%)	482 (21%)	3	1

5 of 482 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	405	LEU
6	E	502	ARG
6	F	551	GLU
6	E	488	ILE
7	G	46	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	E	464	HIS
7	G	98	ASN
6	E	562	ASN
6	F	464	HIS
6	E	265	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	I	24/33 (72%)	2 (8%)	1 (4%)
5	J	26/59 (44%)	1 (3%)	1 (3%)
All	All	50/92 (54%)	3 (6%)	2 (4%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	I	15	G
4	I	23	C
5	J	25	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	I	22	G
5	J	25	G

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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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	$\# Z > 2$
9	GDP	A	1003	10	24,30,30	1.00	1 (4%)	30,47,47	1.25	4 (13%)

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
9	GDP	A	1003	10	-	1/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1003	GDP	C6-N1	-2.77	1.33	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1003	GDP	C3'-C2'-C1'	3.23	105.84	100.98
9	A	1003	GDP	PA-O3A-PB	-2.87	122.99	132.83
9	A	1003	GDP	C5-C6-N1	2.18	117.80	113.95
9	A	1003	GDP	C8-N7-C5	2.17	107.13	102.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

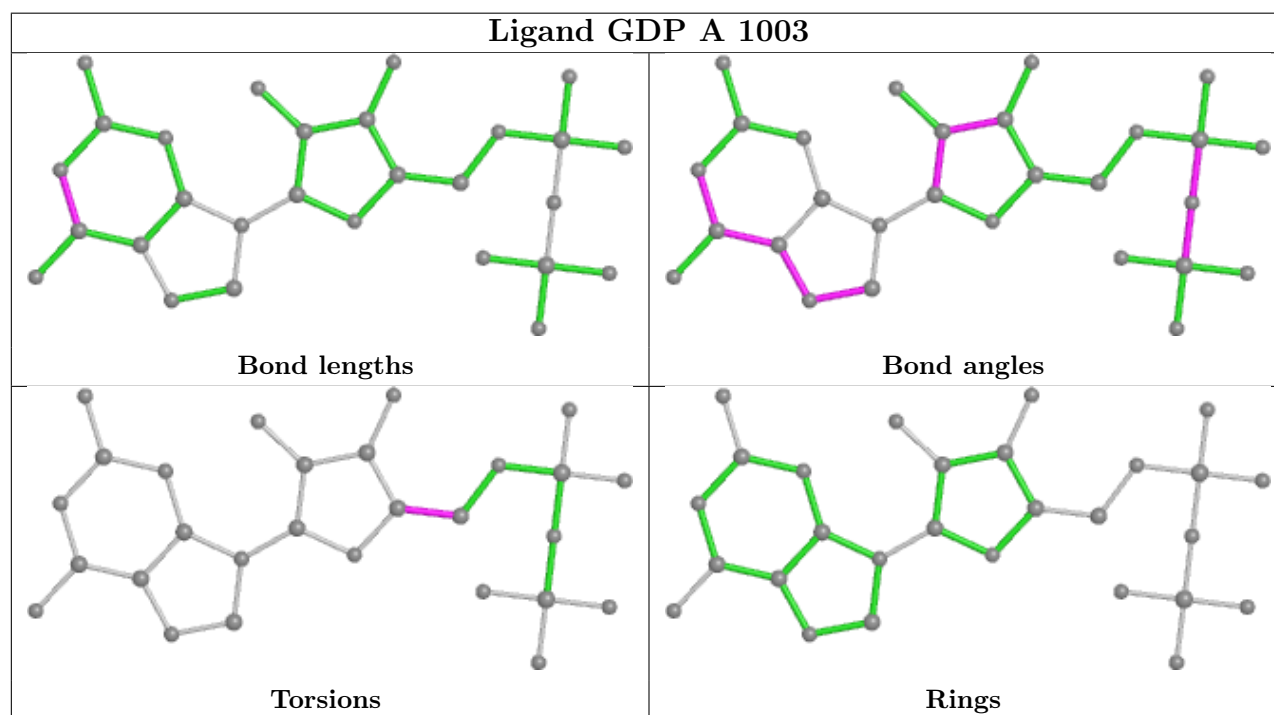
Mol	Chain	Res	Type	Atoms
9	A	1003	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1003	GDP	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 than 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.



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.

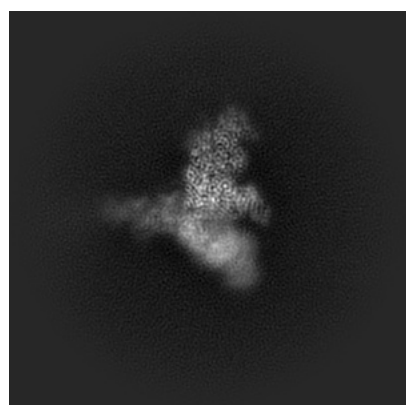
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30504. These allow visual inspection of the internal detail of the map and identification of artifacts.

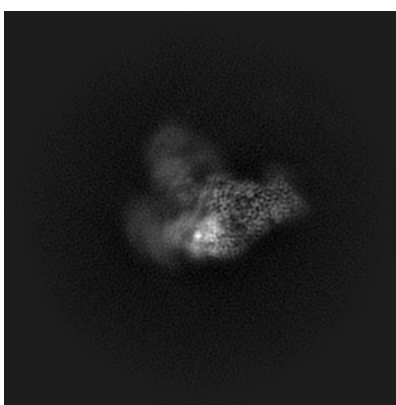
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

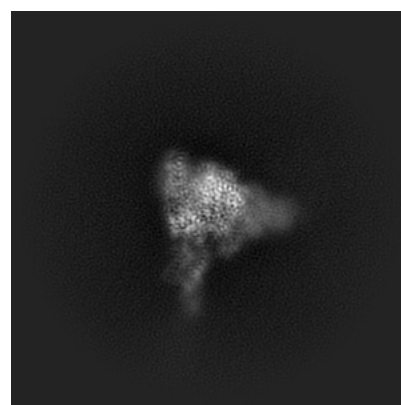
6.1.1 Primary map



X



Y

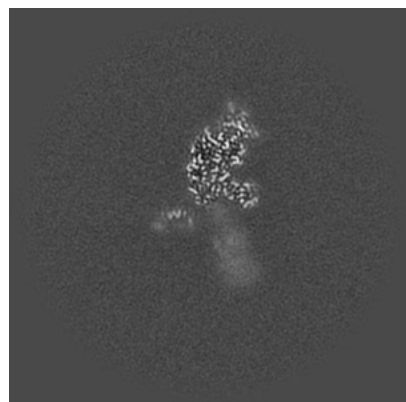


Z

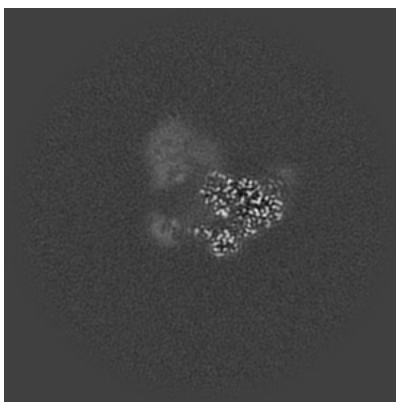
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

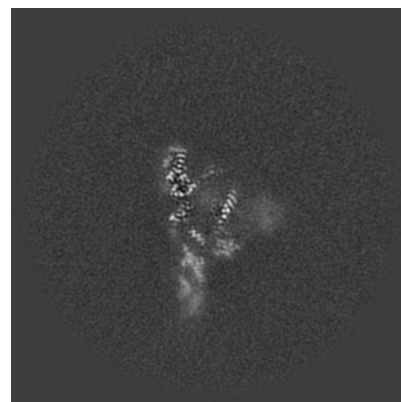
6.2.1 Primary map



X Index: 224



Y Index: 224

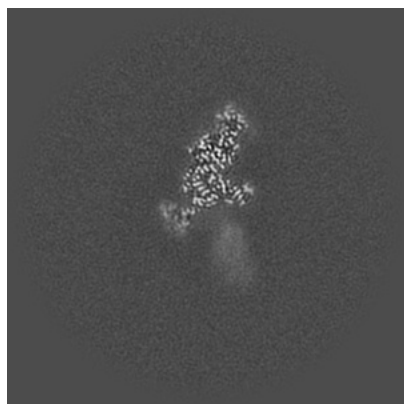


Z Index: 224

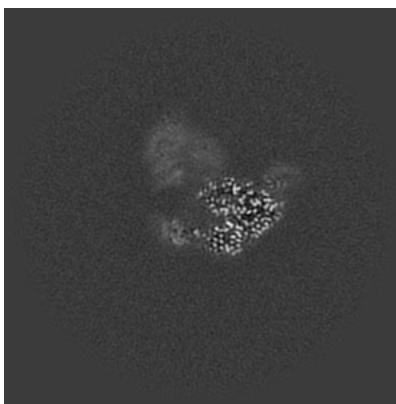
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

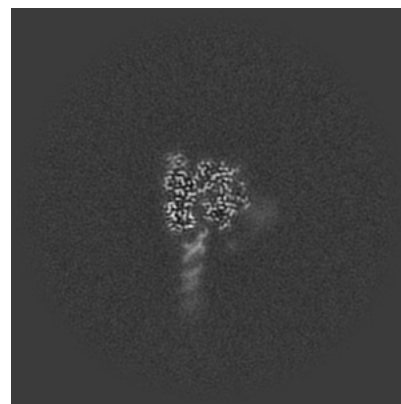
6.3.1 Primary map



X Index: 232



Y Index: 218

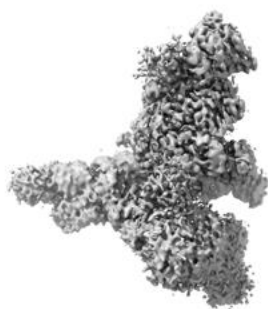


Z Index: 236

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

6.4 Orthogonal surface views [i](#)

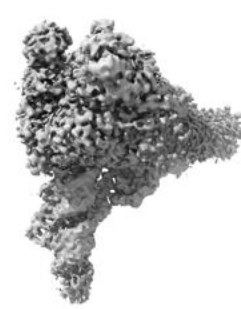
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

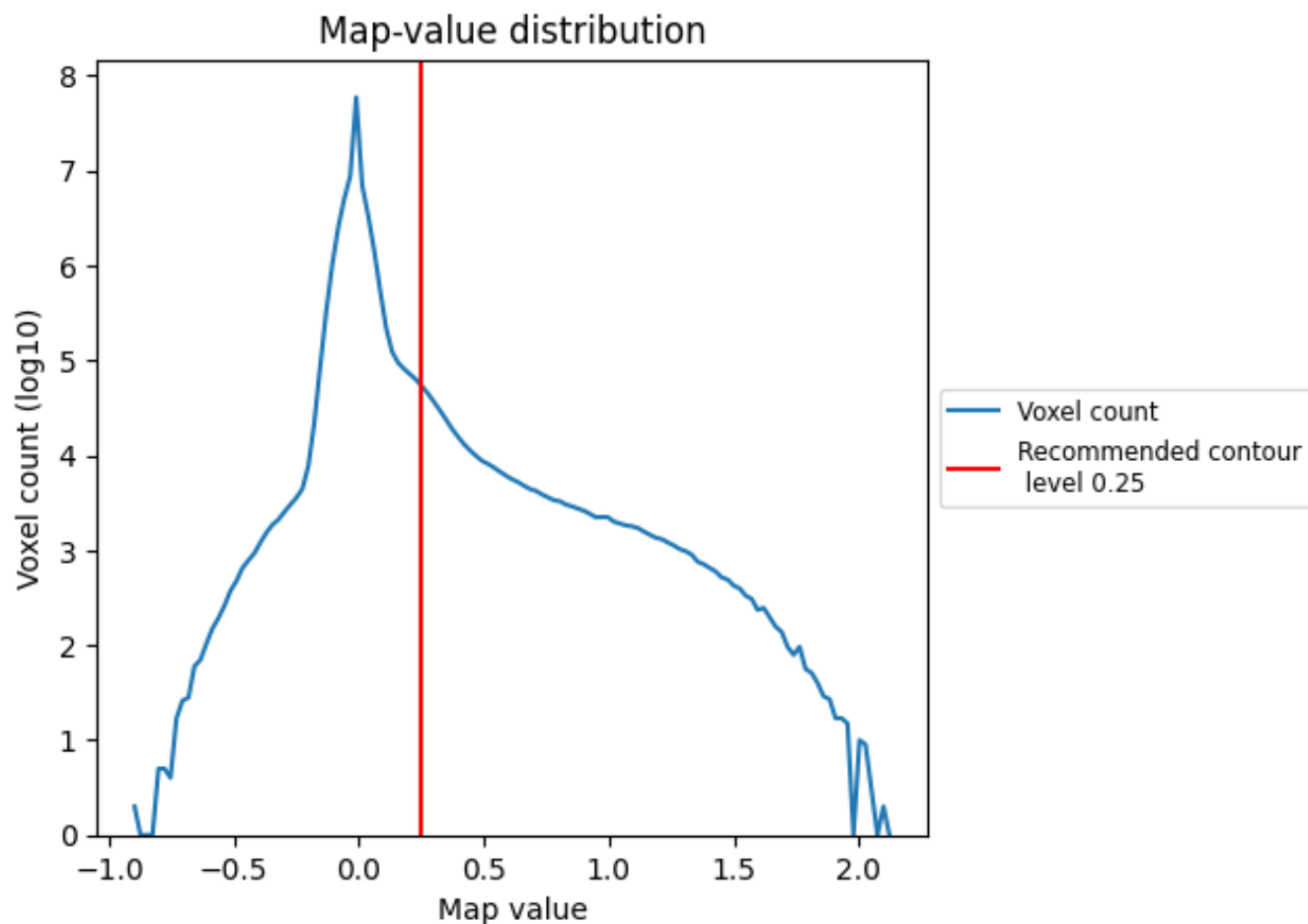
6.5 Mask visualisation

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

7 Map analysis [i](#)

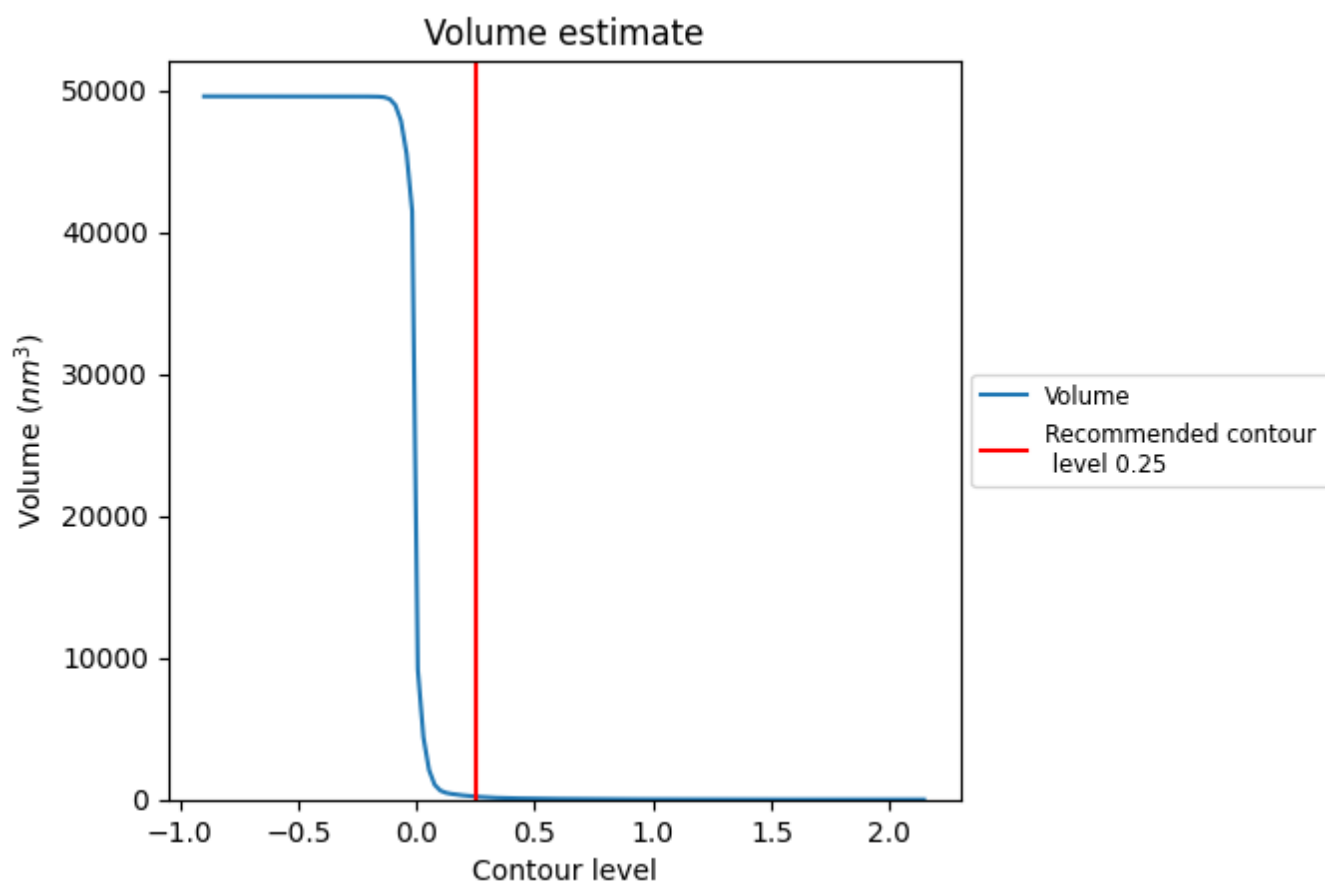
This section contains the results of statistical analysis of the map.

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.

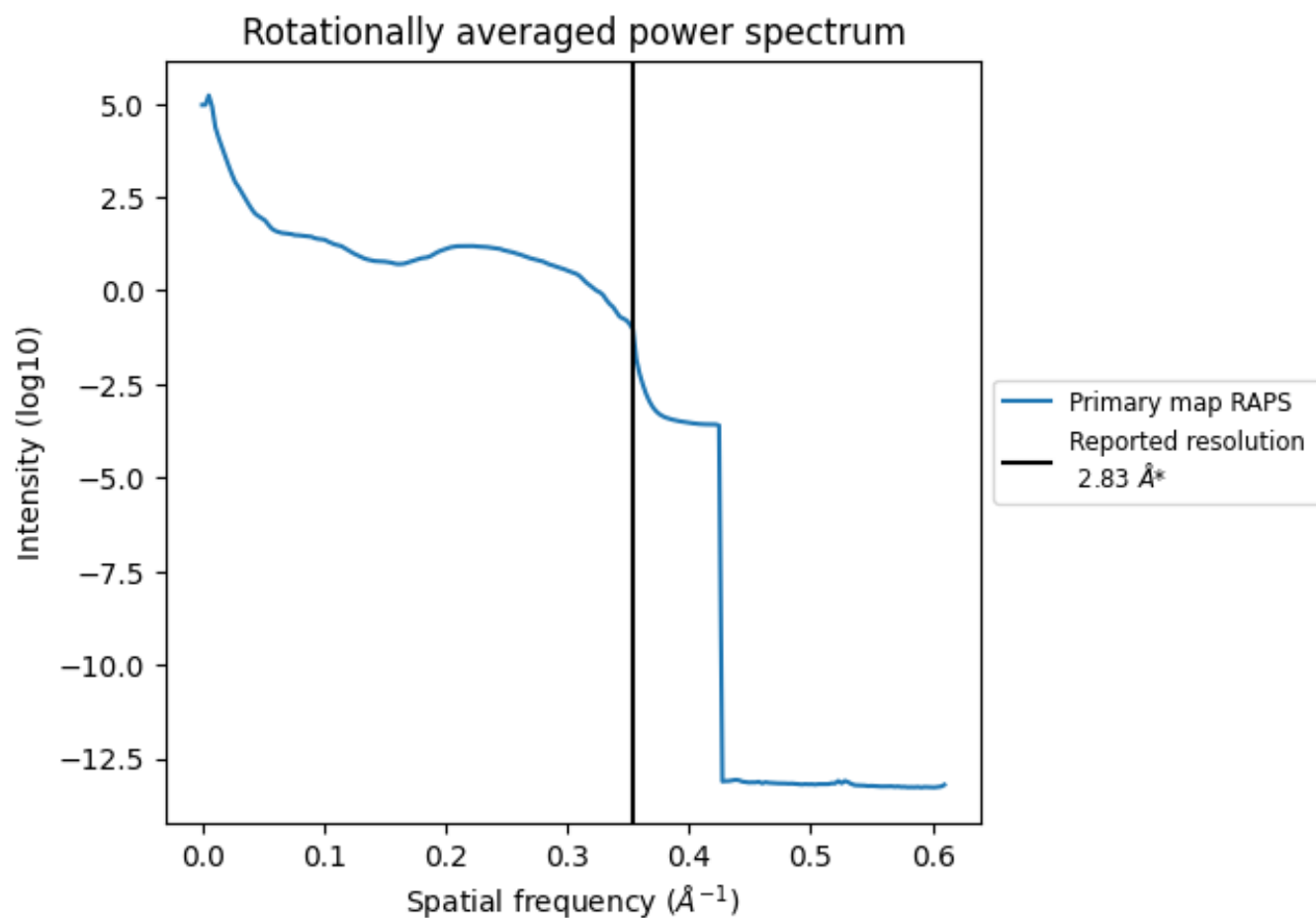
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm³; this corresponds to an approximate mass of 192 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

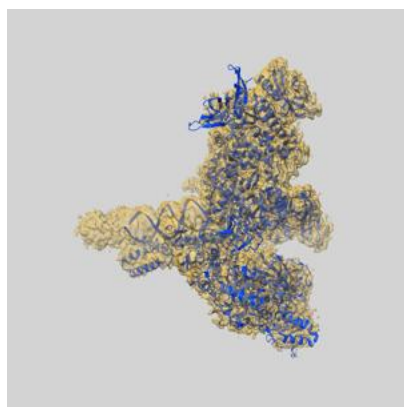
8 Fourier-Shell correlation ⓘ

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

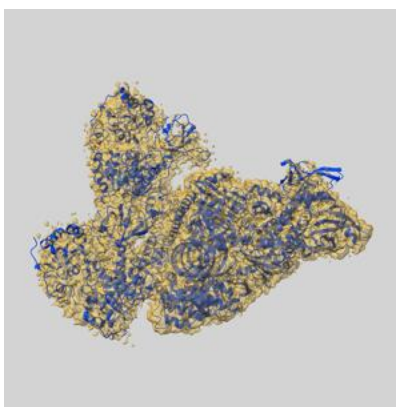
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30504 and PDB model 7CYQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

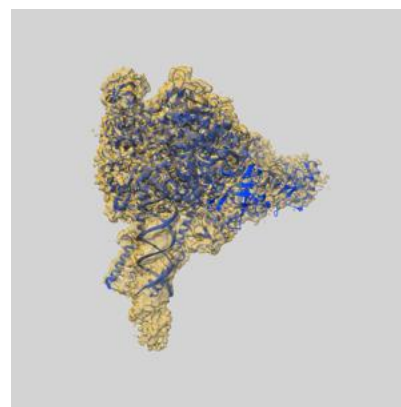
9.1 Map-model overlay [i](#)



X



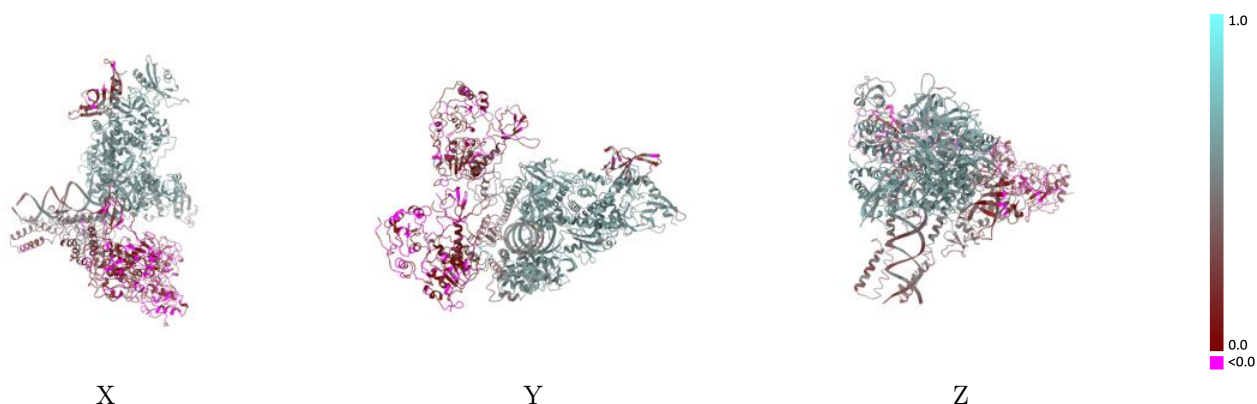
Y



Z

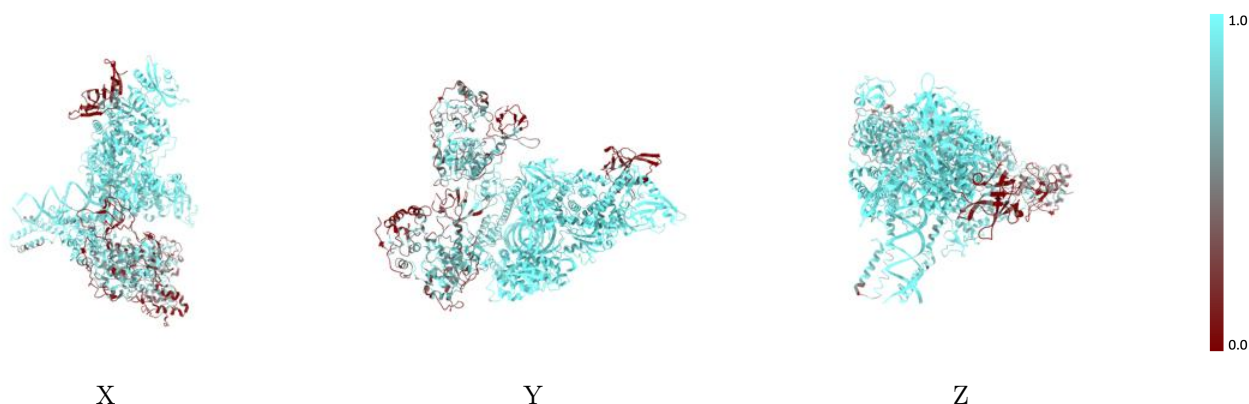
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



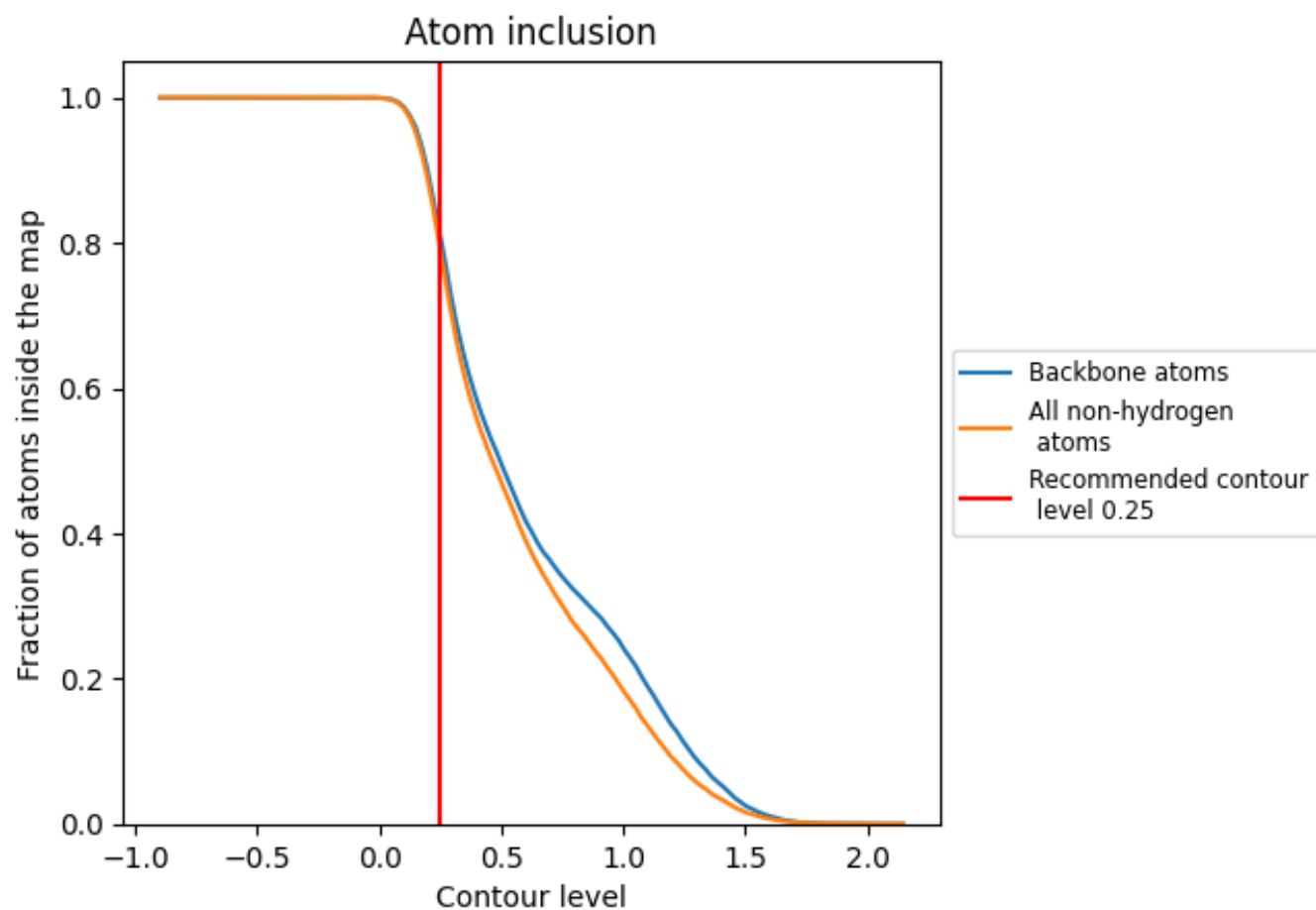
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 79% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7887	<div></div> 0.3840
A	<div></div> 0.9857	<div></div> 0.5900
B	<div></div> 0.9389	<div></div> 0.5000
C	<div></div> 0.9782	<div></div> 0.5660
D	<div></div> 0.9418	<div></div> 0.4740
E	<div></div> 0.6221	<div></div> 0.2140
F	<div></div> 0.5625	<div></div> 0.1140
G	<div></div> 0.2541	<div></div> 0.3280
I	<div></div> 0.9982	<div></div> 0.4550
J	<div></div> 0.9823	<div></div> 0.4770

1.0

0.0

<0.0