



# Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:51 PM JST

PDB ID : 7WPB  
EMDB ID : EMD-32681  
Title : SARS-CoV-2 Omicron Variant RBD complexed with ACE2  
Authors : Yin, W.; Xu, Y.; Xu, P.; Cao, X.; Wu, C.; Gu, C.; He, X.; Wang, X.; Huang, S.; Yuan, Q.; Wu, K.; Hu, W.; Huang, Z.; Liu, J.; Wang, Z.; Jia, F.; Xia, K.; Liu, P.; Wang, X.; Song, B.; Zheng, J.; Jiang, H.; Cheng, X.; Jiang, Y.; Deng, S.; Xu, E.  
Deposited on : 2022-01-23  
Resolution : 2.79 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

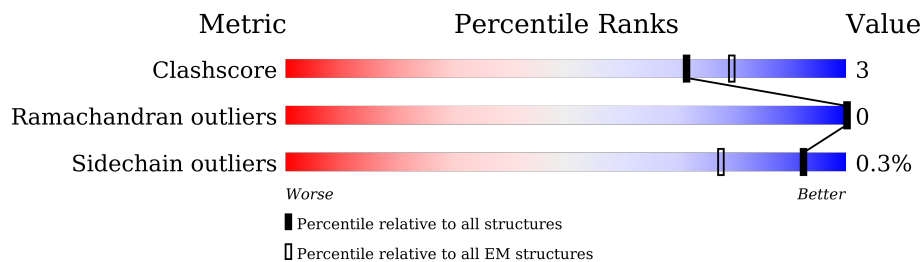
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.79 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  $\geq 3$ , 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	1205	
2	D	805	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6491 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	198	1590	1025	269	288	8	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	93	ILE	THR	variant	UNP P0DTC2
A	140	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	206	ILE	-	insertion	UNP P0DTC2
A	207	VAL	-	insertion	UNP P0DTC2
A	208	ARG	ASN	variant	UNP P0DTC2
A	209	GLU	LEU	variant	UNP P0DTC2
A	210	PRO	VAL	variant	UNP P0DTC2
A	211	GLU	ARG	variant	UNP P0DTC2
A	336	ASP	GLY	variant	UNP P0DTC2
A	368	LEU	SER	variant	UNP P0DTC2
A	370	PRO	SER	variant	UNP P0DTC2
A	372	PHE	SER	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	437	LYS	ASN	variant	UNP P0DTC2
A	443	SER	GLY	variant	UNP P0DTC2
A	474	ASN	SER	variant	UNP P0DTC2
A	475	LYS	THR	variant	UNP P0DTC2
A	481	ALA	GLU	variant	UNP P0DTC2
A	490	ARG	GLN	variant	UNP P0DTC2
A	493	SER	GLY	variant	UNP P0DTC2
A	495	ARG	GLN	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2

*Continued on next page...*

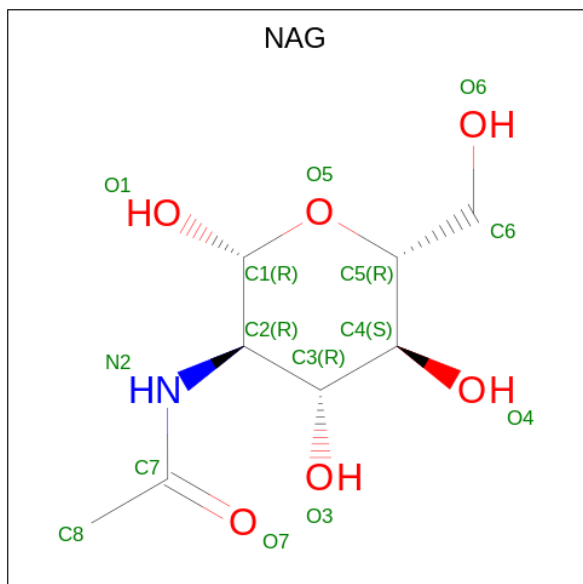
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	HIS	TYR	variant	UNP P0DTC2
A	544	LYS	THR	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	652	TYR	HIS	variant	UNP P0DTC2
A	676	LYS	ASN	variant	UNP P0DTC2
A	678	HIS	PRO	variant	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	680	SER	ARG	engineered mutation	UNP P0DTC2
A	682	SER	ARG	engineered mutation	UNP P0DTC2
A	761	LYS	ASN	variant	UNP P0DTC2
A	793	TYR	ASP	variant	UNP P0DTC2
A	853	LYS	ASN	variant	UNP P0DTC2
A	951	HIS	GLN	variant	UNP P0DTC2
A	966	LYS	ASN	variant	UNP P0DTC2
A	978	PHE	LEU	variant	UNP P0DTC2
A	983	PRO	LYS	engineered mutation	UNP P0DTC2
A	984	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	595	4857	3108	804	916	29	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
3	D	1	Total	C	N	O	0
			42	24	3	15	
3	D	1	Total	C	N	O	0
			42	24	3	15	
3	D	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Cl	0
			1	1	

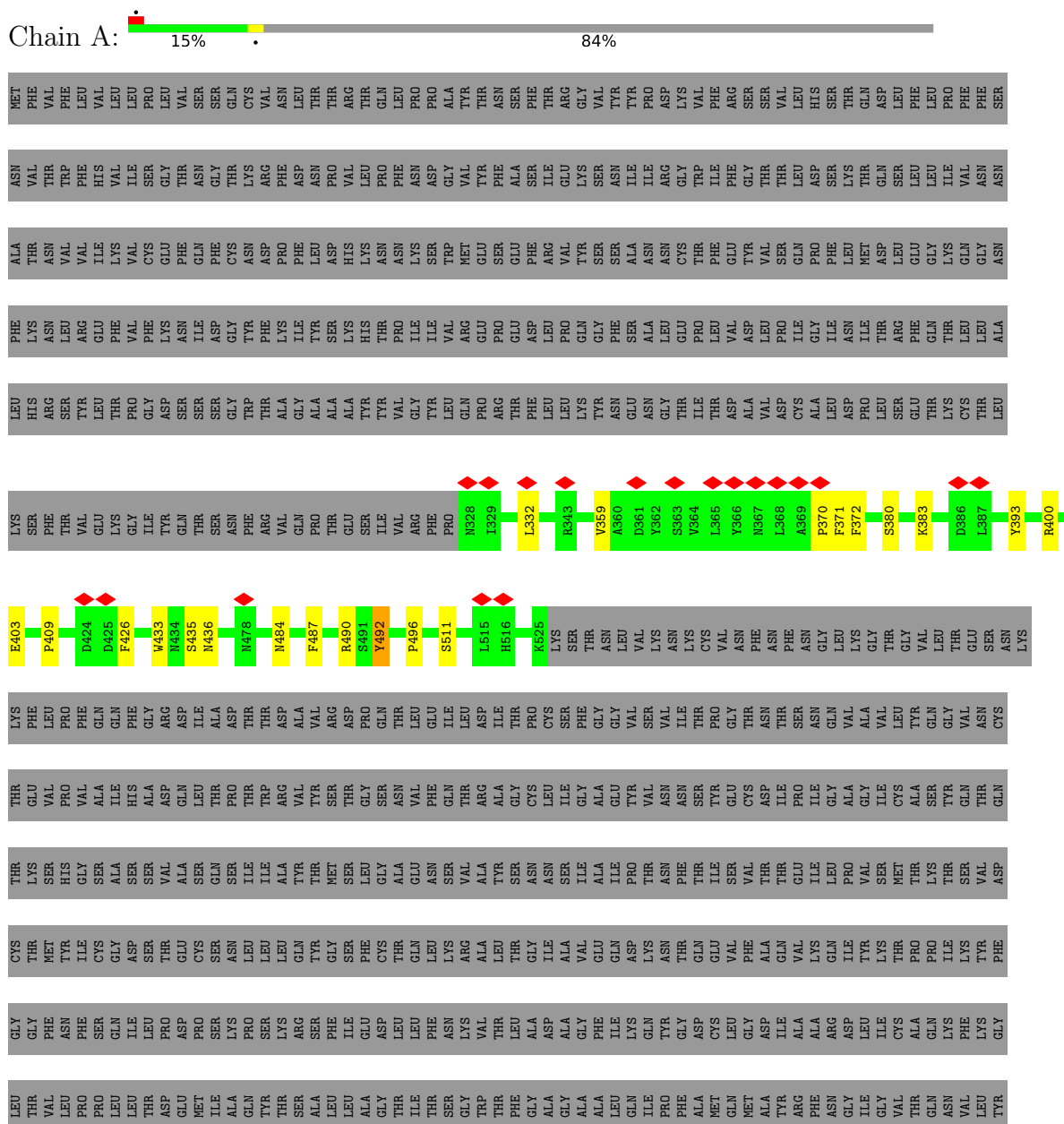
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	D	1	Total	Zn	0
			1	1	

### 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: Spike glycoprotein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5071668	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.389	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.985	Depositor
Minimum map value	-6.563	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.73	Depositor
Map size ( $\text{\AA}$ )	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.824, 0.824, 0.824	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: ZN, CL, 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	0.34	0/1637	0.50	0/2228
2	D	0.30	0/4994	0.46	0/6785
All	All	0.31	0/6631	0.47	0/9013

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1590	0	1526	12	0
2	D	4857	0	4631	33	0
3	D	42	0	39	0	0
4	D	1	0	0	0	0
5	D	1	0	0	0	0
All	All	6491	0	6196	44	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 3.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ASN:HD21	1:A:496:PRO:HA	1.59	0.67
2:D:22:GLU:HG3	2:D:88:ILE:HG23	1.81	0.60
2:D:351:LEU:HB2	2:D:355:ASP:HB3	1.85	0.59
2:D:288:LYS:NZ	2:D:431:ASP:OD2	2.39	0.55
1:A:332:LEU:HD23	1:A:359:VAL:HG13	1.89	0.55
2:D:224:GLU:O	2:D:228:HIS:ND1	2.41	0.54
2:D:460:ARG:NH2	2:D:510:TYR:O	2.38	0.53
2:D:501:ALA:O	2:D:507:SER:OG	2.27	0.53
2:D:431:ASP:OD1	2:D:431:ASP:N	2.43	0.53
2:D:152:MET:O	2:D:161:ARG:NH2	2.42	0.52
2:D:388:GLN:O	2:D:393:ARG:NH1	2.43	0.51
1:A:484:ASN:ND2	2:D:24:GLN:OE1	2.44	0.51
2:D:336:PRO:HB2	2:D:340:GLN:HB3	1.93	0.51
2:D:482:ARG:NH1	2:D:608:THR:O	2.44	0.50
2:D:535:HIS:NE2	2:D:538:PRO:O	2.40	0.49
2:D:155:SER:O	2:D:161:ARG:NH1	2.46	0.48
2:D:25:ALA:HB1	2:D:97:LEU:HD11	1.96	0.48
2:D:53:ASN:O	2:D:58:ASN:ND2	2.44	0.47
1:A:409:PRO:HG3	1:A:426:PHE:HB3	1.96	0.47
2:D:161:ARG:HG3	2:D:265:HIS:HD2	1.80	0.46
2:D:204:ARG:HG2	2:D:222:LEU:HD23	1.97	0.46
2:D:177:ARG:NH1	2:D:470:LYS:O	2.50	0.45
2:D:114:LYS:O	2:D:118:THR:OG1	2.30	0.45
2:D:457:GLU:HG2	2:D:512:PHE:HB3	1.99	0.44
1:A:380:SER:HB3	1:A:383:LYS:HB2	1.99	0.44
2:D:74:LYS:HB3	2:D:74:LYS:HE3	1.87	0.44
2:D:111:ASP:OD1	2:D:111:ASP:N	2.52	0.43
1:A:435:SER:OG	1:A:435:SER:O	2.35	0.43
1:A:393:TYR:HB2	1:A:511:SER:HB3	2.01	0.42
2:D:133:CYS:HA	2:D:141:CYS:HA	2.01	0.42
2:D:261:CYS:HB2	2:D:488:VAL:HB	2.00	0.42
2:D:209:VAL:HG11	2:D:565:PRO:HB3	2.01	0.42
2:D:83:TYR:HA	2:D:84:PRO:HD3	1.89	0.42
1:A:487:PHE:HB3	1:A:490:ARG:HH22	1.84	0.41
2:D:494:ASP:OD1	2:D:494:ASP:N	2.49	0.41
2:D:243:TYR:OH	2:D:247:LYS:NZ	2.41	0.41
2:D:335:ASP:HA	2:D:336:PRO:HD3	1.92	0.41
1:A:400:ARG:HB2	1:A:403:GLU:HG3	2.02	0.41
1:A:370:PRO:HG2	1:A:371:PHE:HD1	1.86	0.41
1:A:403:GLU:OE1	1:A:492:TYR:OH	2.30	0.41
2:D:245:ARG:NH1	2:D:603:PHE:O	2.53	0.41
1:A:371:PHE:HA	1:A:433:TRP:HB3	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:MET:HG2	2:D:256:ILE:HB	2.02	0.40
2:D:47:SER:HA	2:D:62:MET:HG3	2.03	0.40

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	196/1205 (16%)	184 (94%)	12 (6%)	0	100	100
2	D	593/805 (74%)	581 (98%)	12 (2%)	0	100	100
All	All	789/2010 (39%)	765 (97%)	24 (3%)	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	173/1053 (16%)	171 (99%)	2 (1%)	71	92
2	D	526/711 (74%)	526 (100%)	0	100	100
All	All	699/1764 (40%)	697 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	PHE
1	A	492	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	471	GLN
1	A	474	ASN
1	A	478	ASN
2	D	101	GLN
2	D	159	ASN
2	D	239	HIS
2	D	300	GLN
2	D	472	GLN
2	D	505	HIS
2	D	508	ASN
2	D	531	GLN
2	D	556	ASN
2	D	586	ASN
2	D	601	ASN

### 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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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
3	NAG	D	903	2	14,14,15	0.46	0	17,19,21	1.04	2 (11%)
3	NAG	D	902	2	14,14,15	0.34	0	17,19,21	0.74	1 (5%)
3	NAG	D	901	2	14,14,15	0.44	0	17,19,21	0.60	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	D	903	2	-	3/6/23/26	0/1/1/1
3	NAG	D	902	2	-	2/6/23/26	0/1/1/1
3	NAG	D	901	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	903	NAG	C2-N2-C7	3.05	127.24	122.90
3	D	902	NAG	C1-O5-C5	2.25	115.23	112.19
3	D	901	NAG	C1-O5-C5	2.11	115.05	112.19
3	D	903	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	903	NAG	O5-C5-C6-O6
3	D	902	NAG	C8-C7-N2-C2
3	D	902	NAG	O7-C7-N2-C2
3	D	903	NAG	C4-C5-C6-O6
3	D	901	NAG	C4-C5-C6-O6
3	D	901	NAG	O5-C5-C6-O6
3	D	903	NAG	C3-C2-N2-C7

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.

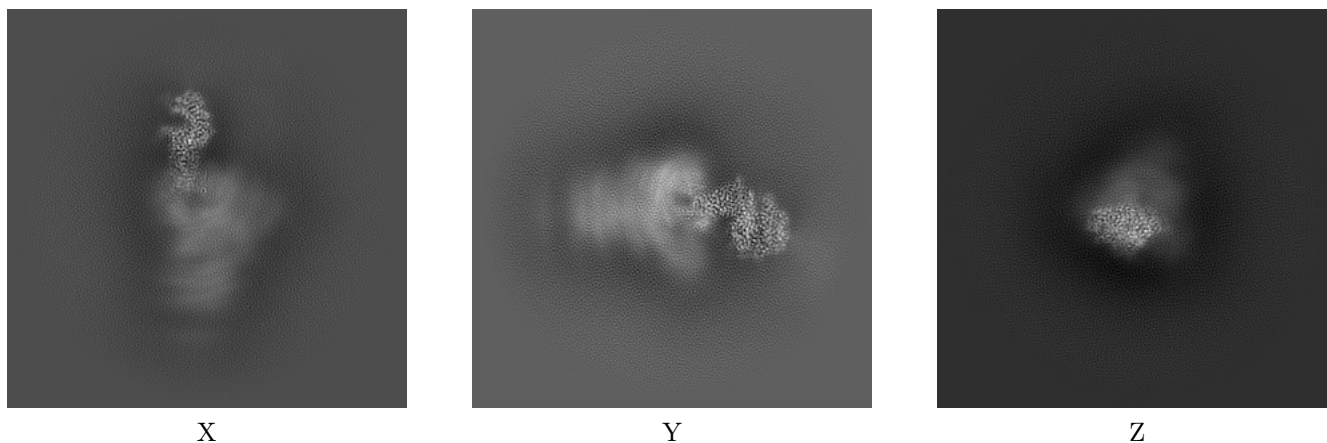
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32681. 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](#)

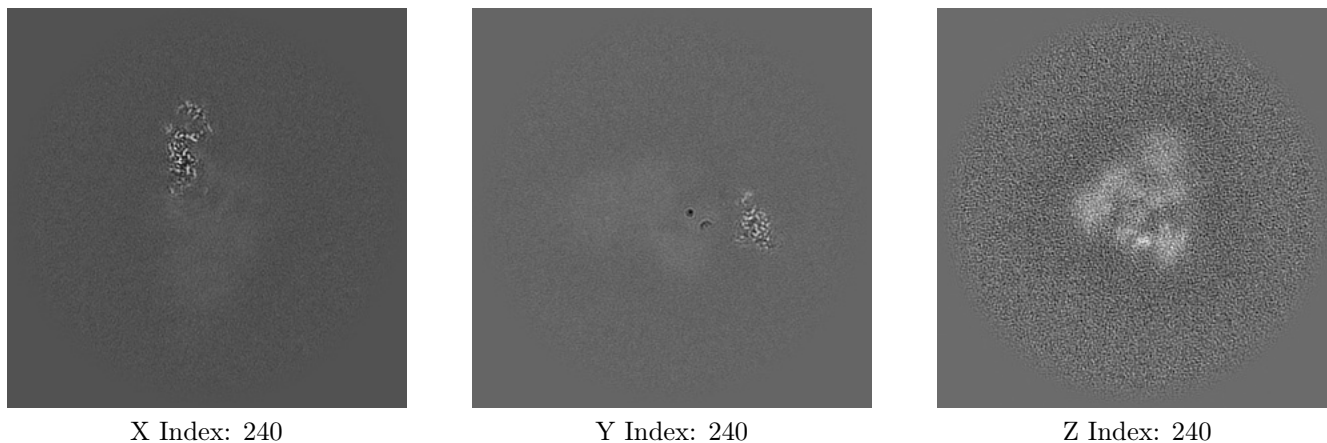
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

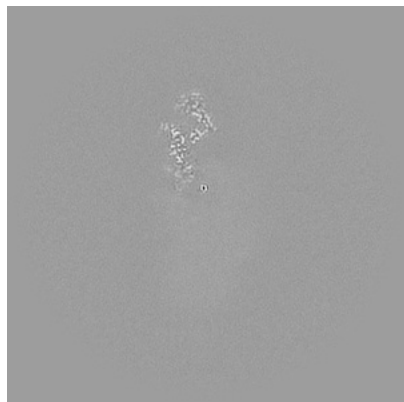
#### 6.2.1 Primary map



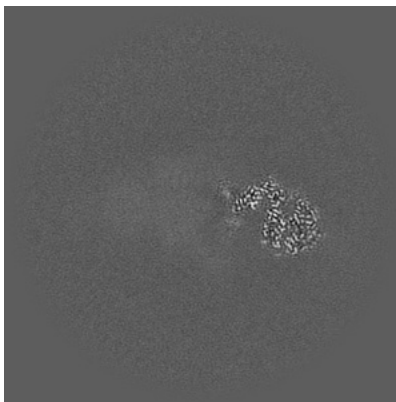
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

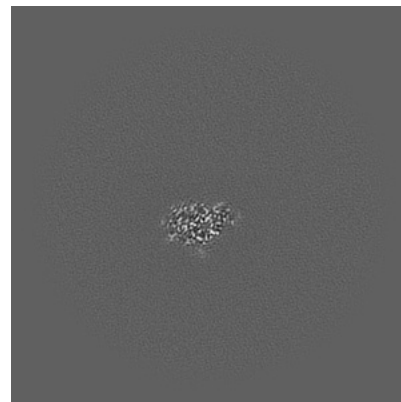
### 6.3.1 Primary map



X Index: 234



Y Index: 222



Z Index: 326

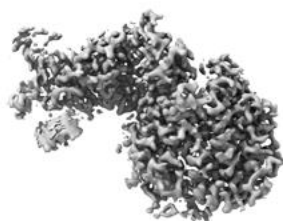
The images above show the largest variance slices of the map in three orthogonal directions.

## 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 0.73. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



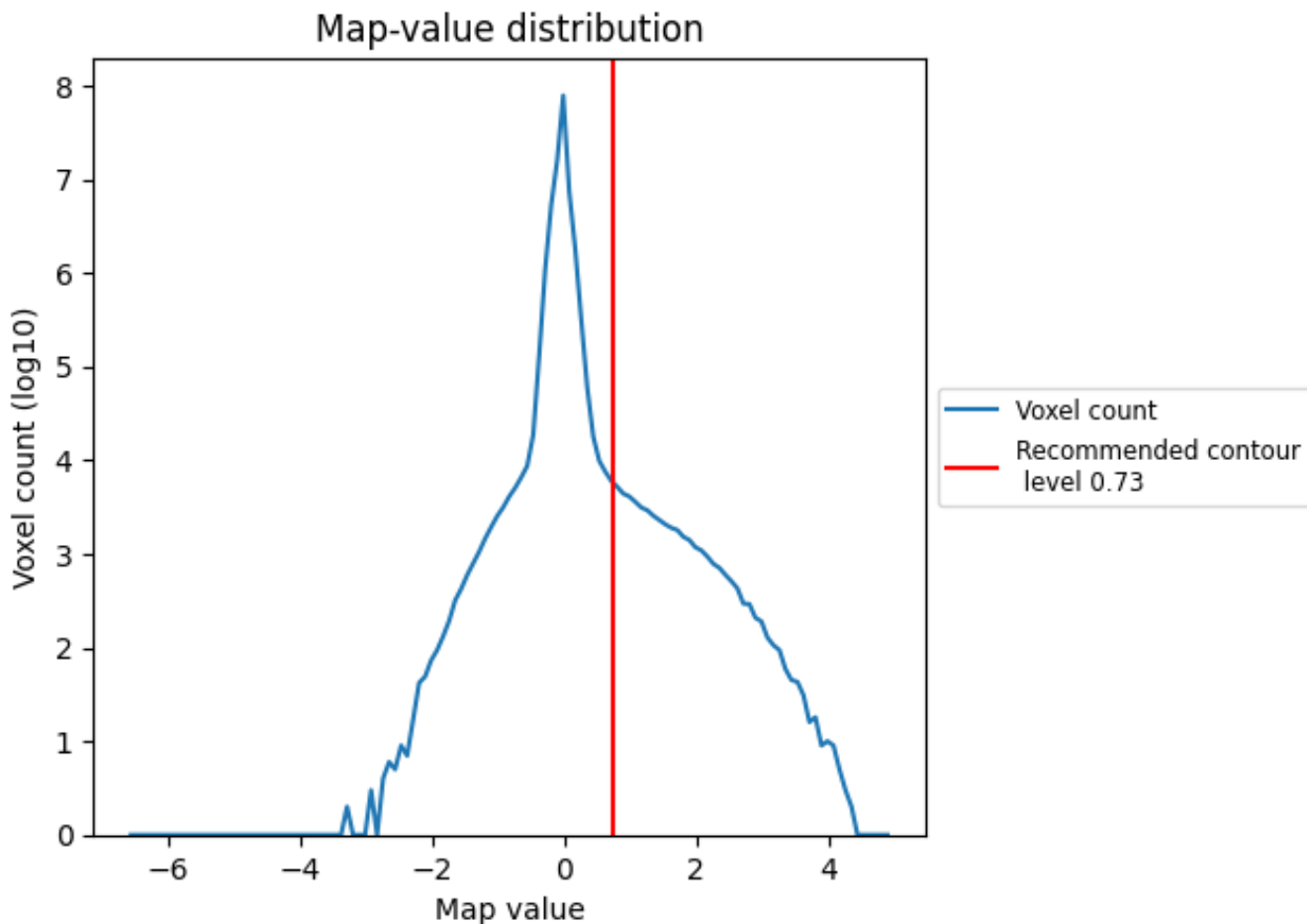
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

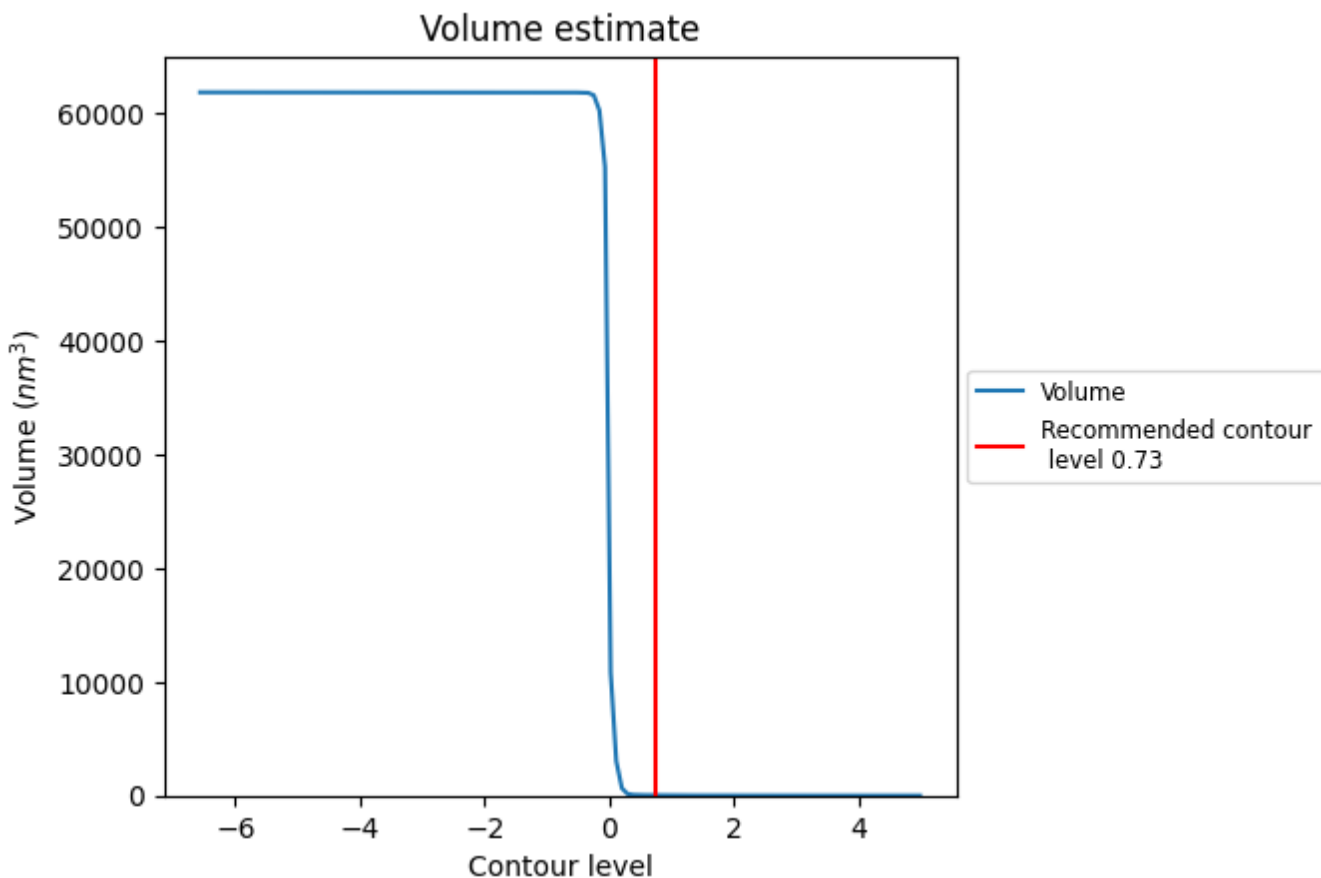
This section contains the results of statistical analysis of the map.

### 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.

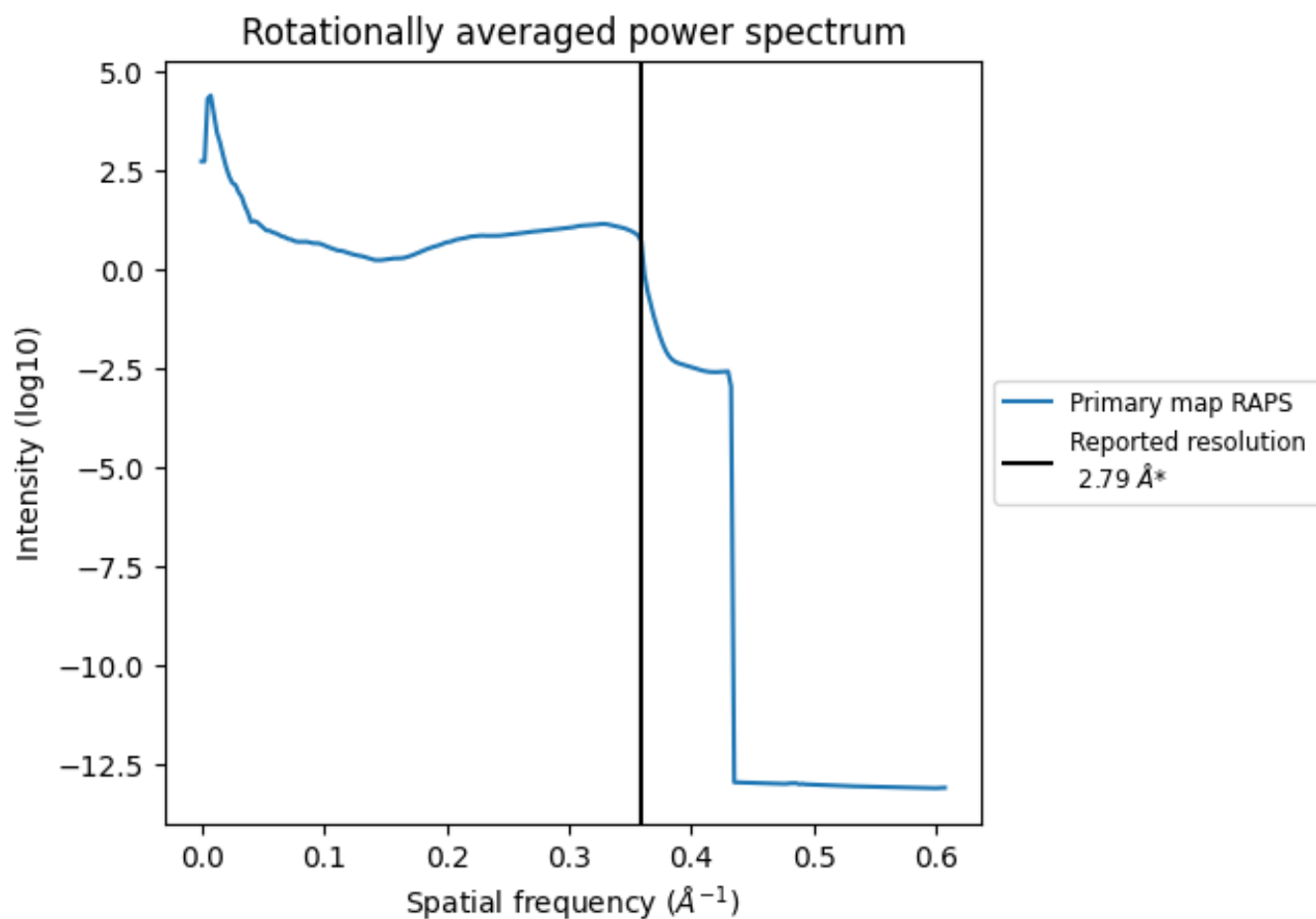
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm<sup>3</sup>; this corresponds to an approximate mass of 25 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  $0.358 \text{\AA}^{-1}$

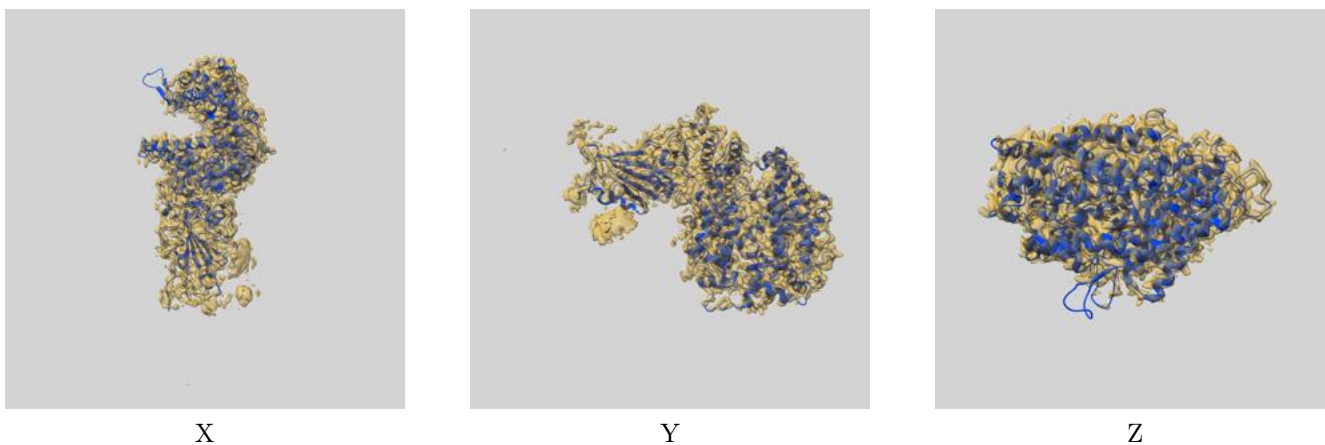
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

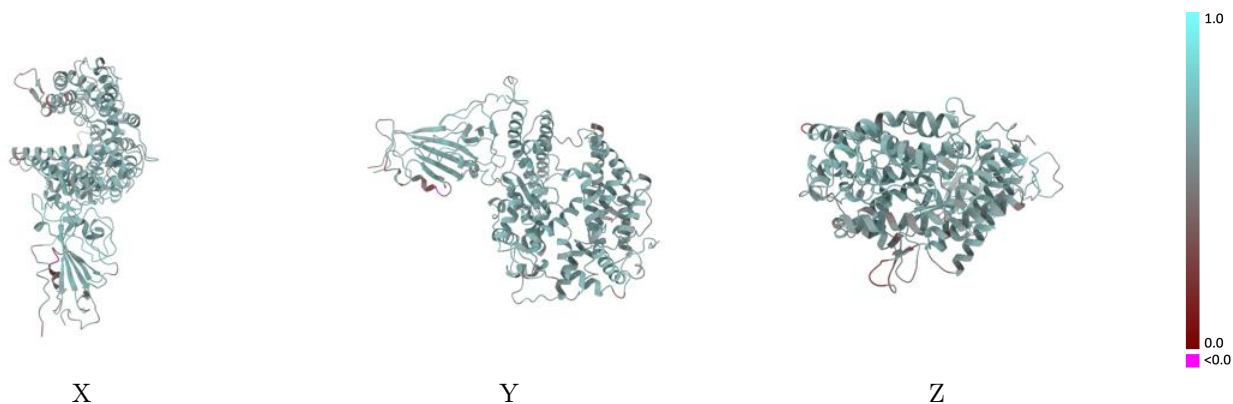
This section contains information regarding the fit between EMDB map EMD-32681 and PDB model 7WPB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



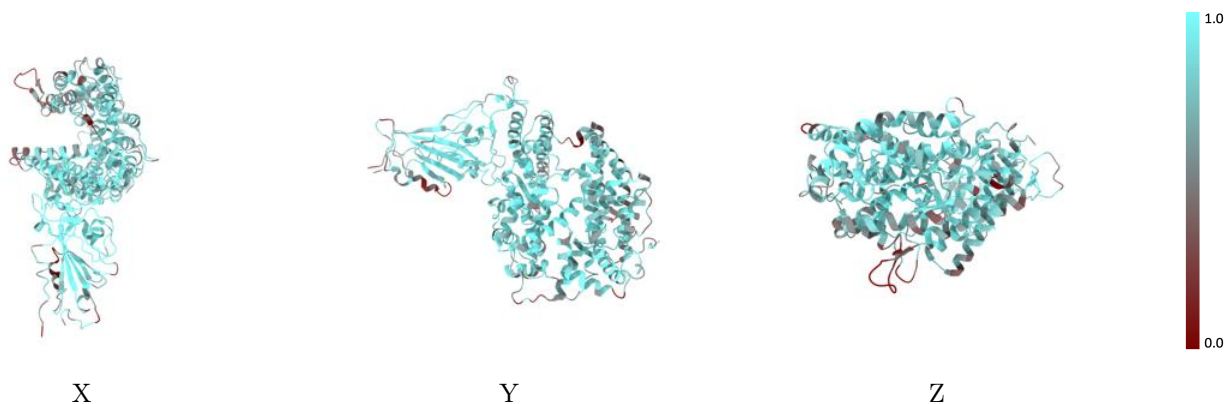
The images above show the 3D surface view of the map at the recommended contour level 0.73 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



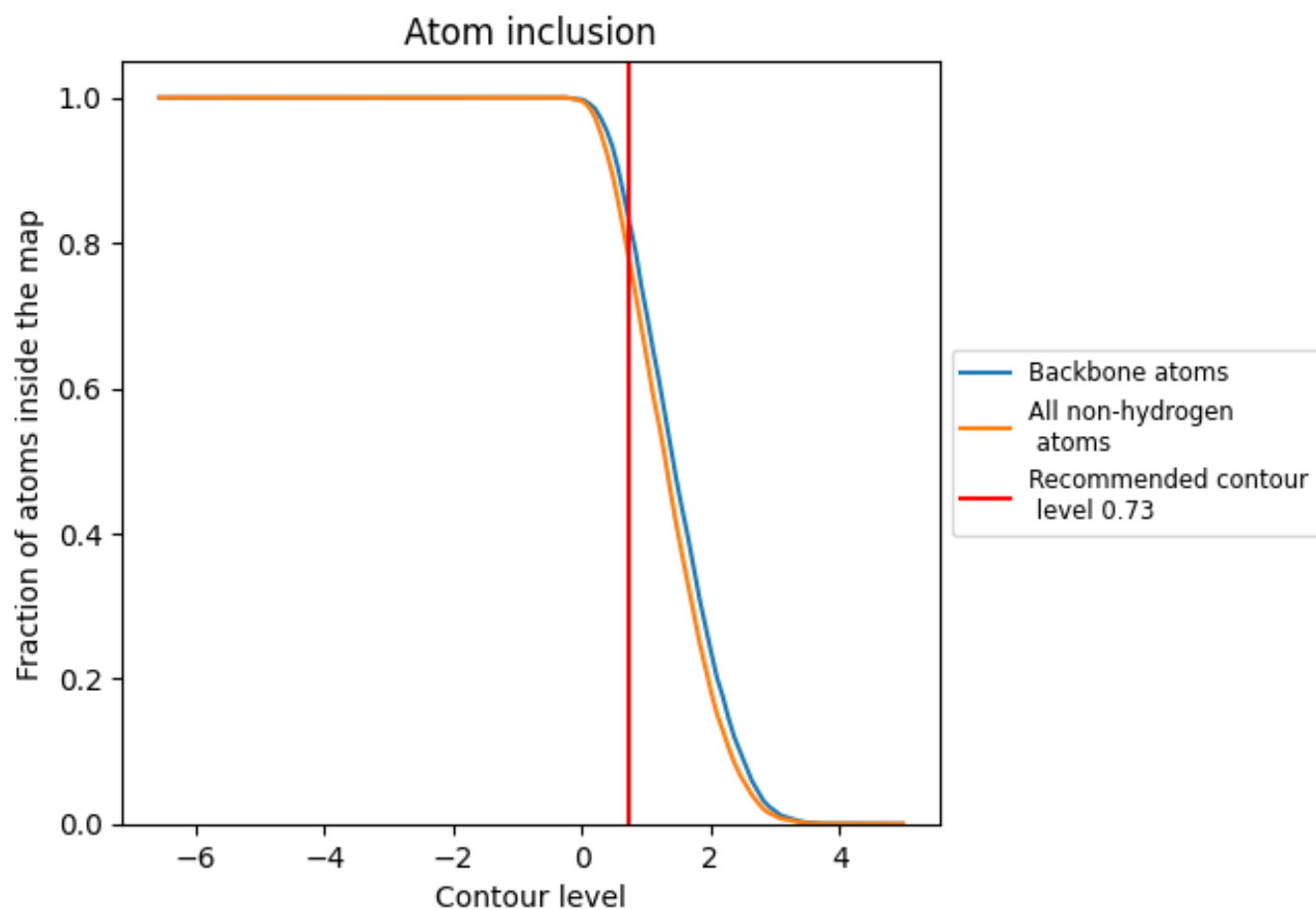
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.73).

## 9.4 Atom inclusion [i](#)







At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.73) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7780	 0.5990
A	 0.7911	 0.5920
D	 0.7737	 0.6020

