



## wwPDB EM Validation Summary Report ⓘ

Nov 6, 2025 – 06:21 PM JST

PDB ID : 9UEL / pdb\_00009uel  
EMDB ID : EMD-64085  
Title : Local refinement of NTD and RBD domains of SARS-CoV2 KP.3.1.1 spike protein  
Authors : He, M.Z.  
Deposited on : 2025-04-08  
Resolution : 3.37 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](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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

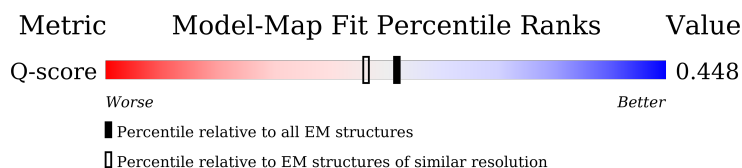
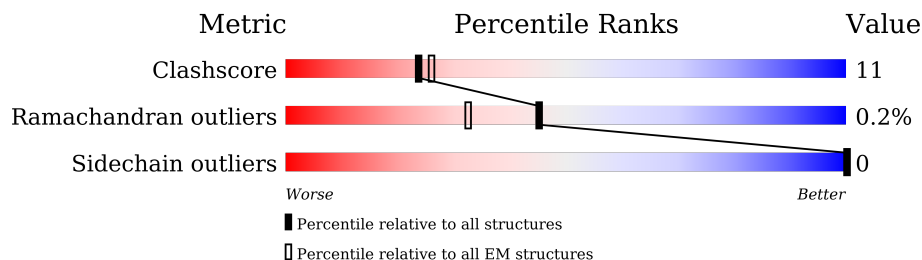
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.37 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14287 ( 2.87 - 3.87 )

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	1305	

## 2 Entry composition [i](#)

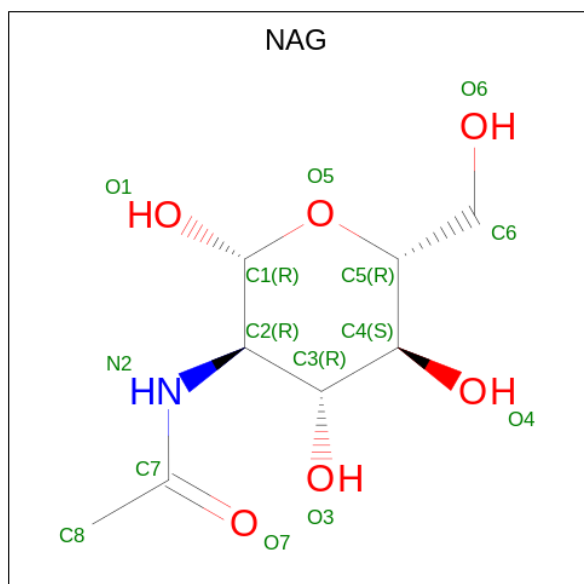
There are 2 unique types of molecules in this entry. The entry contains 4485 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SARS-CoV2 KP.3.1.1 spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	576	4387	2807	717	844	19	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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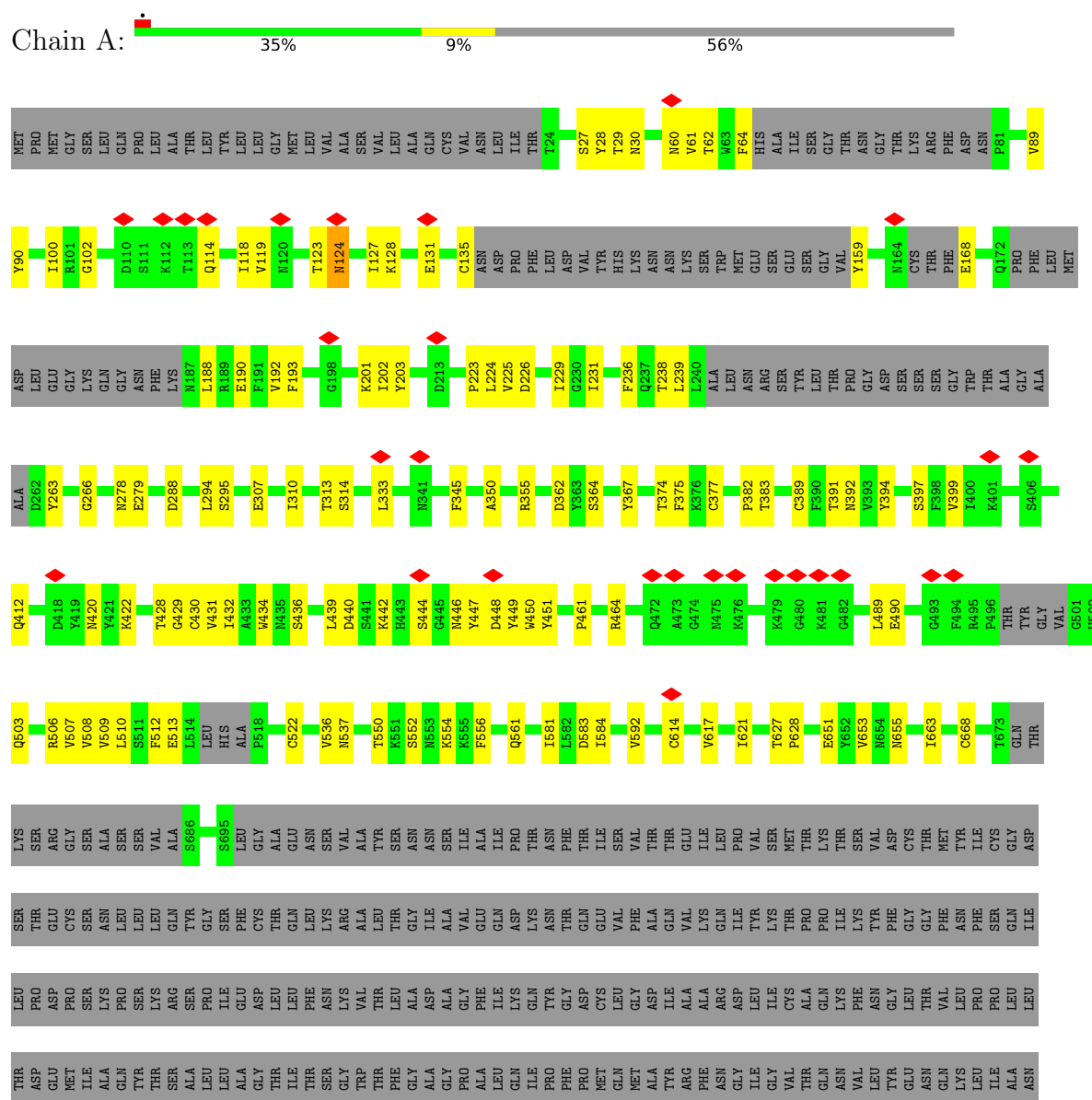
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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

### 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: SARS-CoV2 KP.3.1.1 spike glycoprotein



PHE	LYS	LEU	GLN	GLY	PRO	GLN
GLU	ASP	GLY	ARG	TYR	PRO	PHE
ALA	GLY	ASN	ASN	HIS	GLU	ASN
GLN	GLU	ILE	PHE	LEU	ALA	SER
LYS	TRP	SER	TYR	MET	GUJ	ALA
ILE	VAL	GLY	GLU	SER	VAL	ILE
PHE	PHE	ILE	PRO	PHE	GLN	GLY
TRP	LEU	ASN	GLN	PRO	ILE	LYS
HIS	SER	ALA	ILE	GLN	ASP	ILE
GLU	THR	SER	ILE	SER	ARG	GLN
HIS	PHE	VAL	THR	ALA	LEU	ASP
HIS	LEU	VAL	THR	PRO	ILE	SER
HIS	ASN	ASN	ASP	HIS	THR	LEU
HIS	GLY	ILE	GLY	GLY	ARG	PHE
HIS	LEU	GLN	THR	VAL	ARG	SER
HIS	GLU	LYS	PHE	VAL	LEU	THR
HIS	VAL	GLU	VAL	PHE	GLN	PRO
HIS	LEU	ILE	SER	LEU	SER	SER
	PHE	ASP	GLY	LEU	SER	ALA
	GLN	ARG	ASN	HIS	LEU	ALA
	GLY	LEU	CYS	VAL	GLN	LYS
	PRO	ASN	ASP	TYR	THR	GLY
	GLY	GLU	VAL	VAL	VAL	LEU
	GLY	VAL	VAL	PRO	THR	GLN
	TRP	ALA	ILE	ALA	GLN	ASP
	SER	LYS	GLY	GLN	GLN	VAL
	HIS	ASN	ILE	GLU	LEU	VAL
	PRO	LEU	VAL	ASN	ILE	ASN
	Gln	ASN	ASN	LYS	ARG	HIS
	PHE	GLU	ASN	PHE	ALA	ASN
	GLU	SER	THR	THR	GLU	GLN
	LYS	ILE	VAL	ALA	ILE	ALA
	GLY	ILE	TYR	ALA	ILE	ALA
	GLY	ASP	ASP	PRO	ARG	LEU
	GLY	LEU	PRO	ALA	ALA	ASN
	SER	GLN	LEU	ILE	SER	THR
	GLY	GLU	GLN	CYS	ALA	LEU
	GLY	LEU	LEU	HIS	ASN	VAL
	GLY	GLY	GLU	ASP	LEU	LYS
	SER	LYS	LEU	GLY	ALA	GLN
	GLY	TYR	ASP	LYS	ALA	LEU
	GLY	GLU	SER	ALA	THR	SER
	ALA	GLN	PHE	LYS	LYS	SER
	TRP	SER	GLY	PRO	MET	LYS
	SER	GLY	GLU	ARG	SER	PHE
	HIS	TYR	LEU	GUJ	GUJ	GLY
	PRO	ILE	ASP	GLY	CYS	ALA
	GLN	PRO	LYS	VAL	VAL	ILE
	PHE	GLU	TYR	VAL	LEU	SER
	GLU	ALA	PHE	PHE	GLY	SER
	LYS	PRO	LYS	SER	GLN	VAL
	GLY	ASN	ASN	LYS	LEU	VAL
	GLY	ASP	HIS	GLY	ARG	ASN
	SER	GLY	THR	THR	ASP	ASP
	GLY	GLN	THR	THR	VAL	ILE
	LEU	ALA	PRO	TRP	PHE	LEU
	ASN	TYR	ASP	PHE	SER	ARG
	ASP	VAL	VAL	LEU	CYS	GLY
	ILE	ASP	THR	THR	LYS	LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.547	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.347	Depositor
Map size ( $\text{\AA}$ )	304.0, 304.0, 304.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.76, 0.76, 0.76	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: 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	0.18	0/4491	0.43	0/6129

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	4387	0	4090	93	0
2	A	98	0	91	1	0
All	All	4485	0	4181	93	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 11.

The worst 5 of 93 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:64:PHE:HB2	1:A:263:TYR:HB2	1.58	0.86
1:A:389:CYS:HA	1:A:522:CYS:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LYS:HD3	1:A:444:SER:H	1.50	0.77
1:A:61:VAL:HG13	1:A:62:THR:H	1.48	0.77
1:A:123:THR:O	1:A:124:ASN:HB2	1.92	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	558/1305 (43%)	473 (85%)	84 (15%)	1 (0%)	44 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	ASN

### 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	473/1129 (42%)	473 (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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	ASN
1	A	537	ASN
1	A	560	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	1405	1	14,14,15	0.72	0	17,19,21	1.82	2 (11%)
2	NAG	A	1407	1	14,14,15	0.73	0	17,19,21	0.93	0
2	NAG	A	1401	1	14,14,15	0.74	0	17,19,21	0.79	0
2	NAG	A	1406	1	14,14,15	0.72	0	17,19,21	0.88	0
2	NAG	A	1403	1	14,14,15	0.66	0	17,19,21	0.99	1 (5%)
2	NAG	A	1404	1	14,14,15	0.72	0	17,19,21	0.81	0
2	NAG	A	1402	1	14,14,15	0.78	0	17,19,21	1.11	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
2	NAG	A	1405	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1407	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1406	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1404	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1402	1	-	0/6/23/26	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(°)
2	A	1405	NAG	C1-O5-C5	5.89	120.18	112.19
2	A	1405	NAG	C3-C4-C5	-2.92	105.03	110.24
2	A	1402	NAG	C1-O5-C5	2.74	115.90	112.19
2	A	1403	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1403	NAG	C8-C7-N2-C2
2	A	1403	NAG	O7-C7-N2-C2
2	A	1406	NAG	C8-C7-N2-C2
2	A	1406	NAG	O7-C7-N2-C2
2	A	1407	NAG	C8-C7-N2-C2

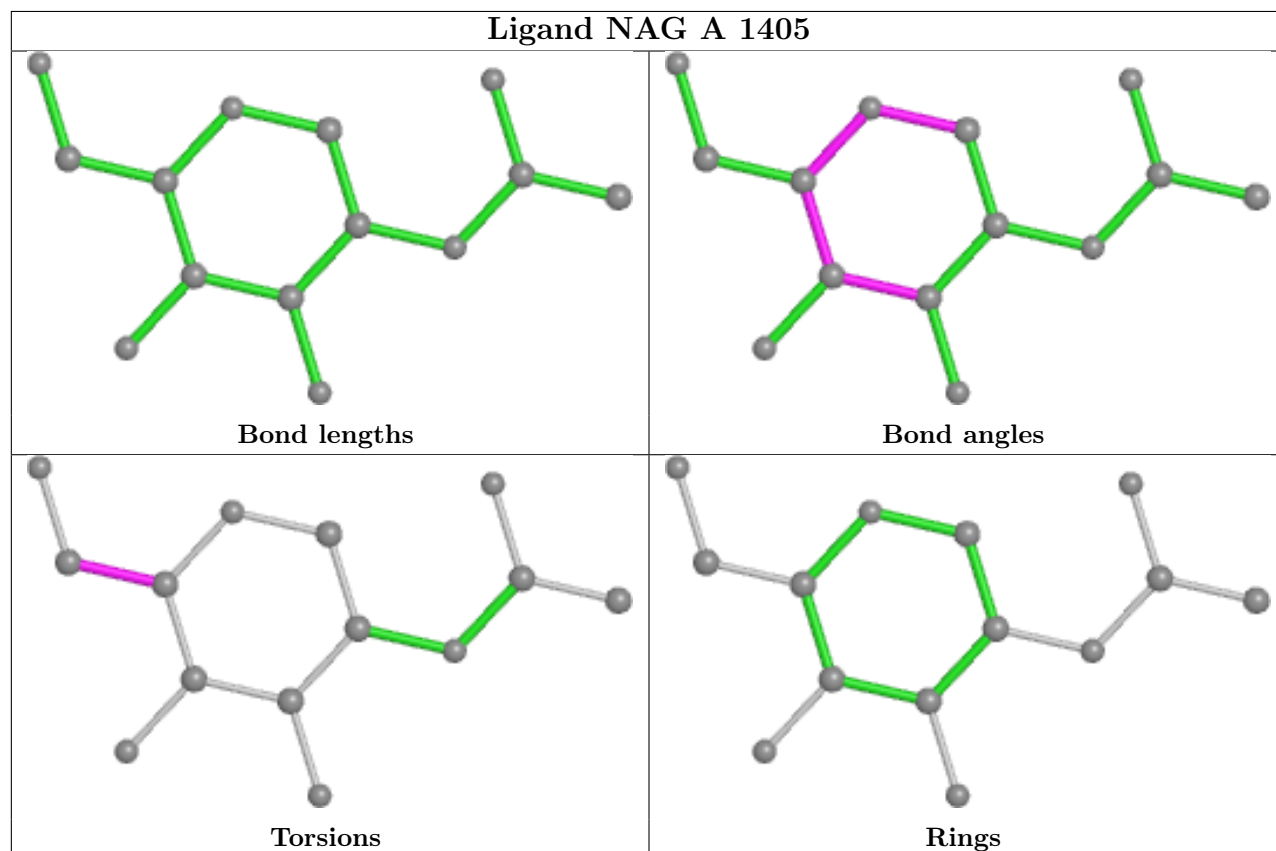
There are no ring outliers.

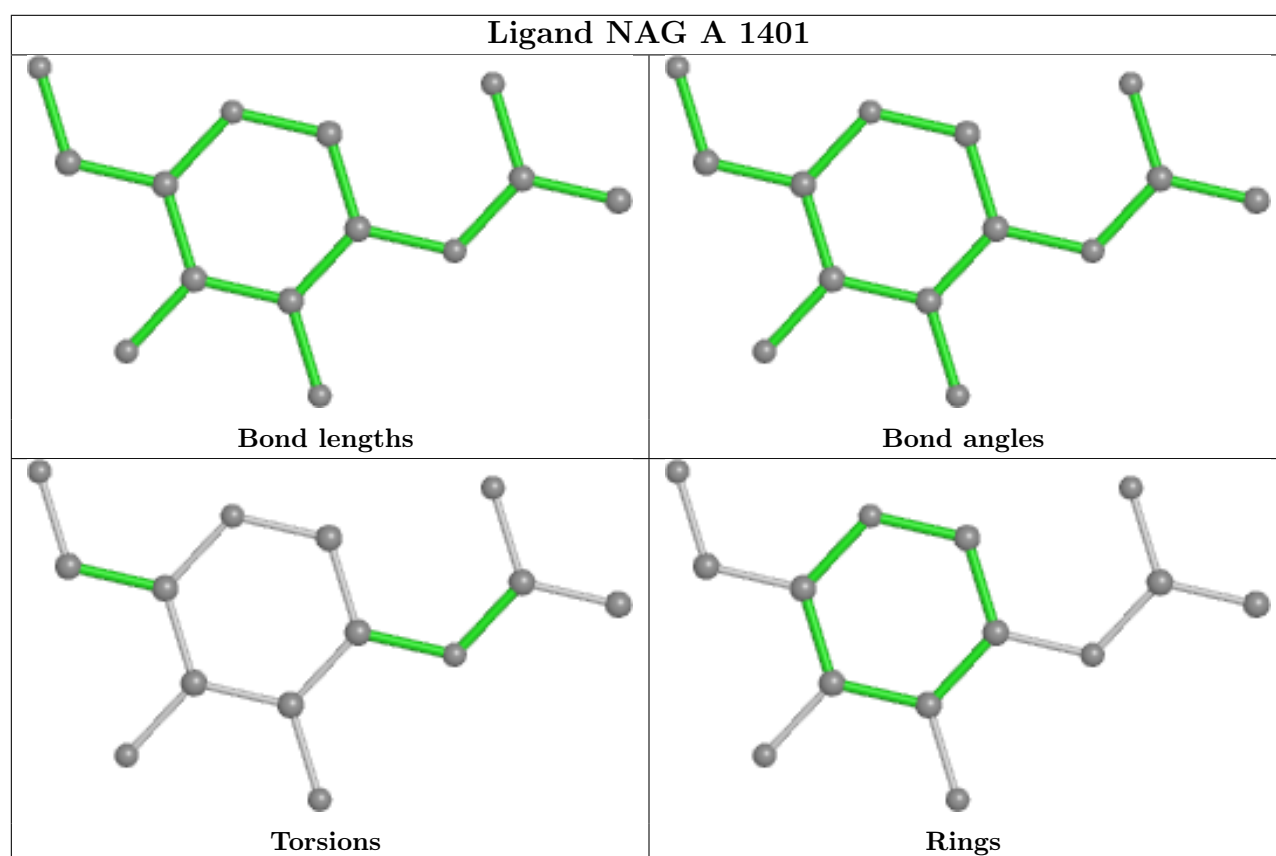
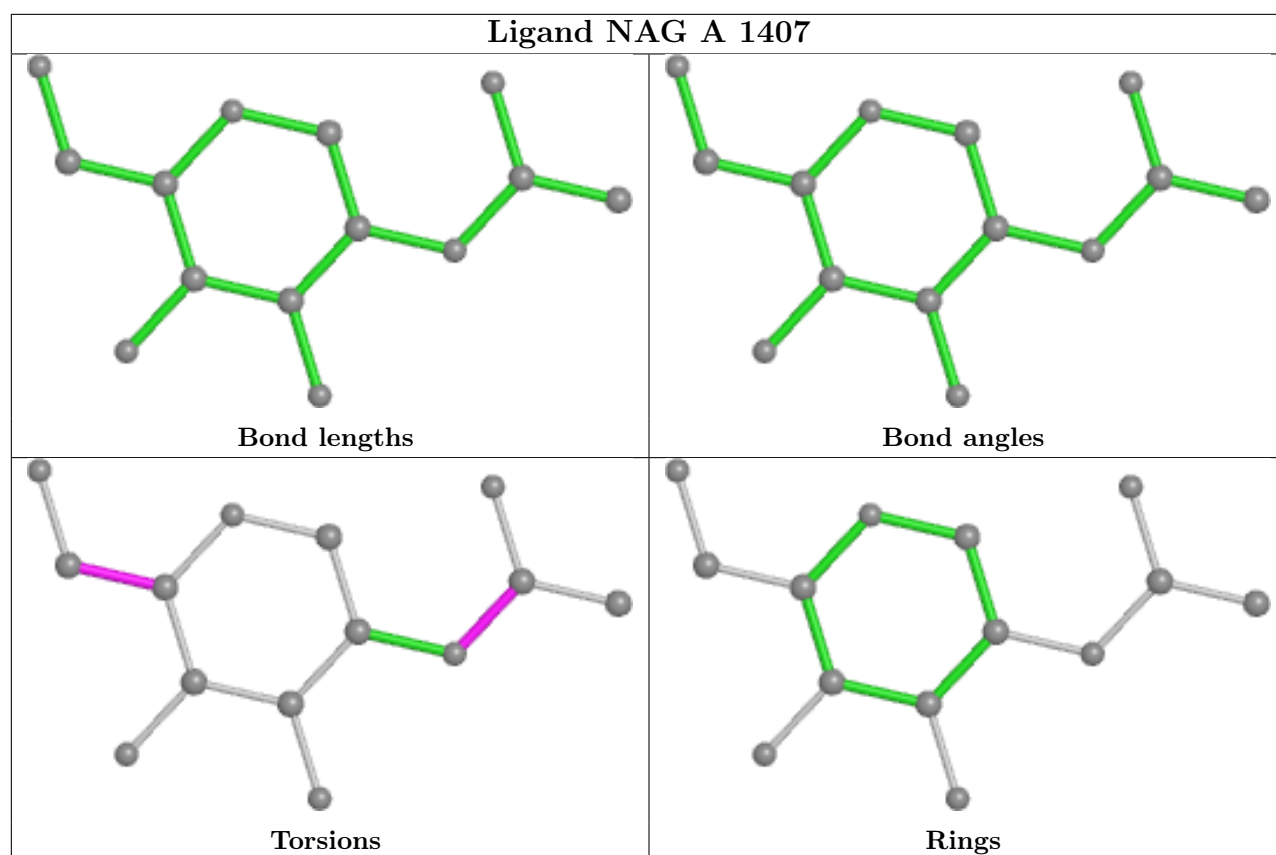
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1407	NAG	1	0

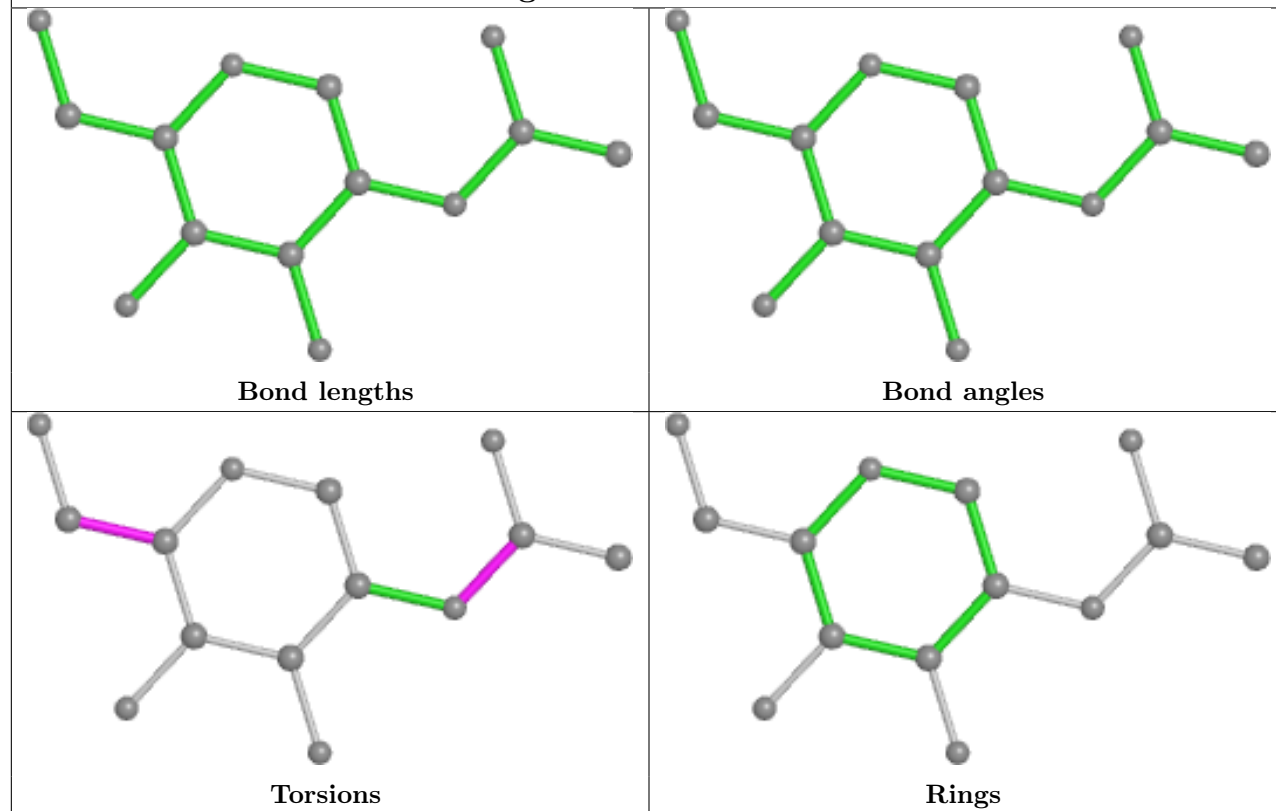
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

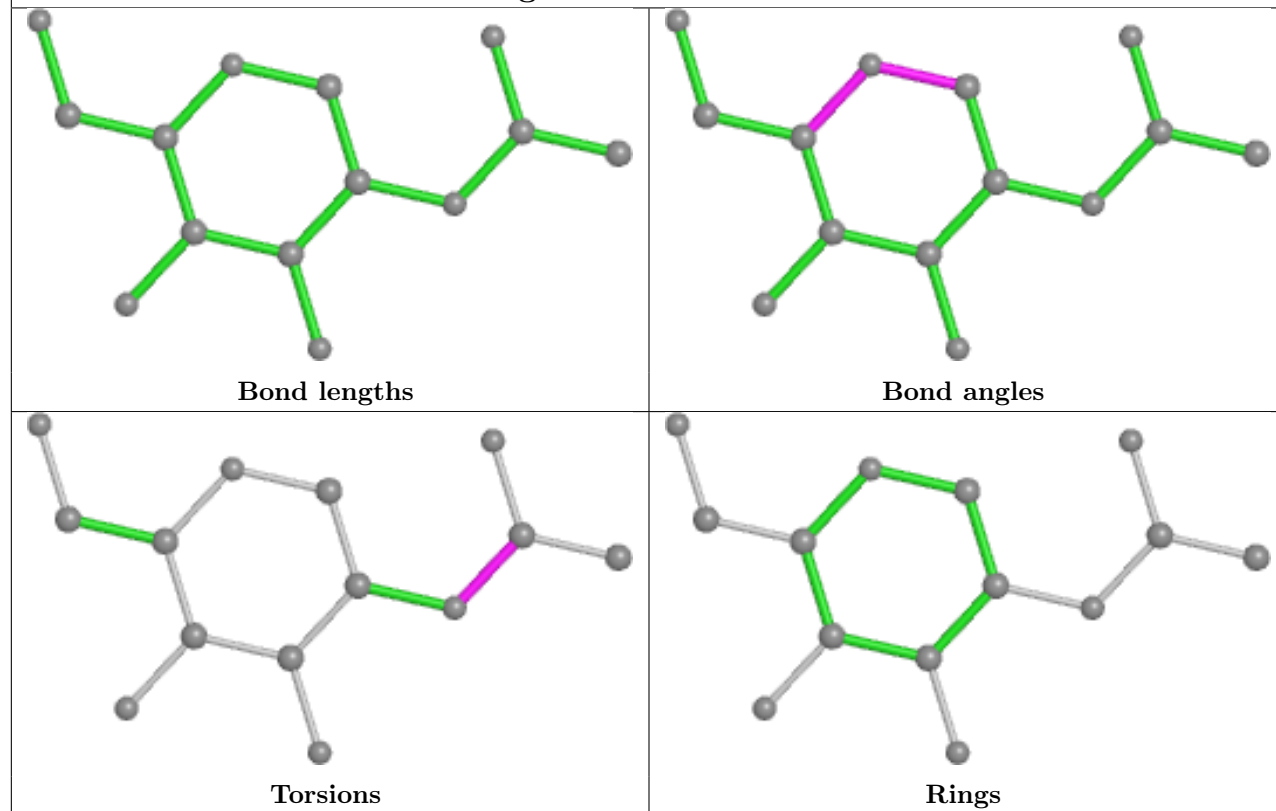


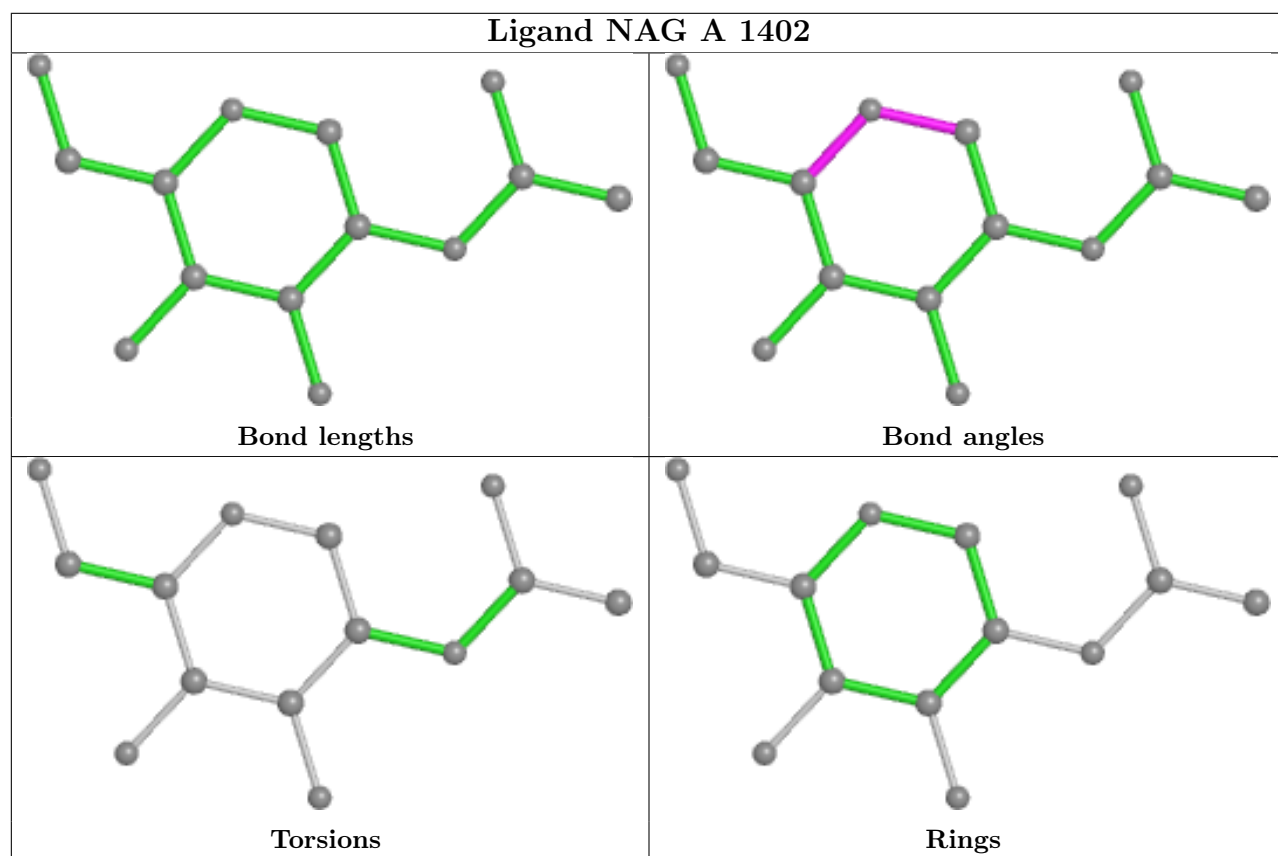
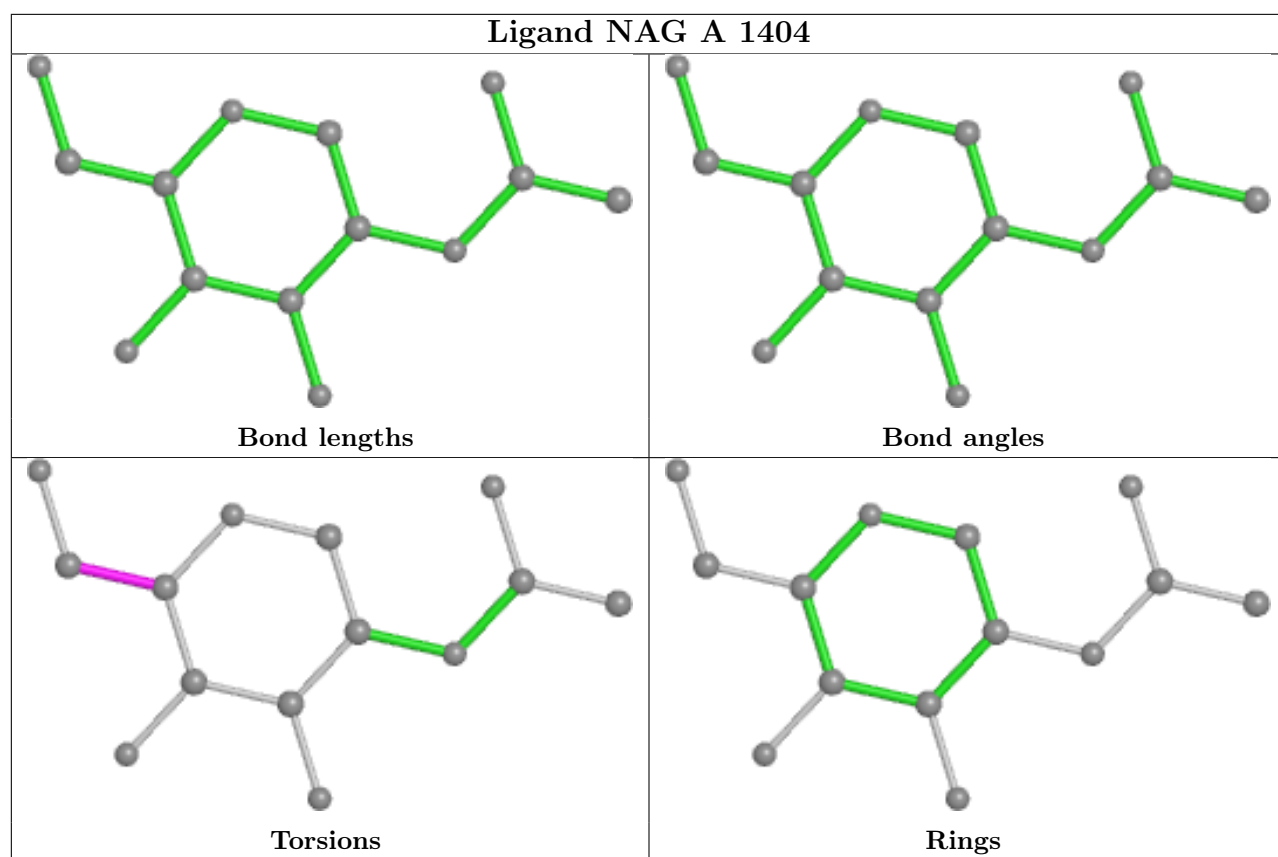


## Ligand NAG A 1406



## Ligand NAG A 1403





## 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.



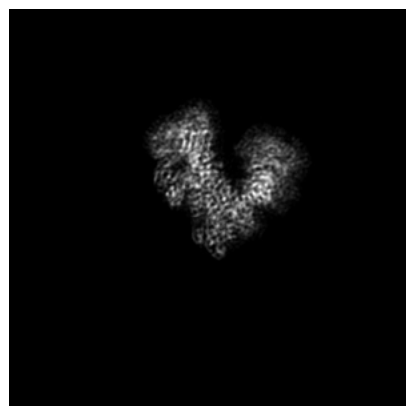
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64085. These allow visual inspection of the internal detail of the map and identification of artifacts.

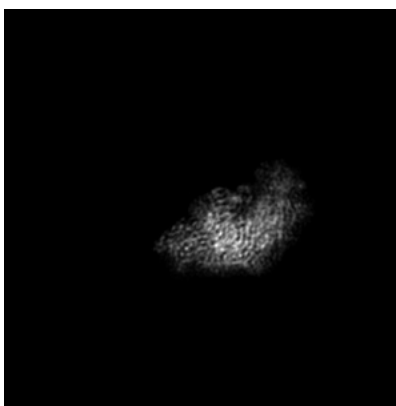
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

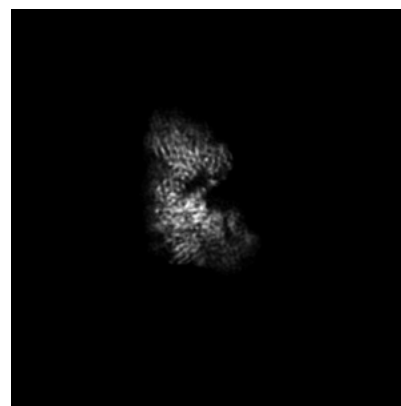
#### 6.1.1 Primary map



X

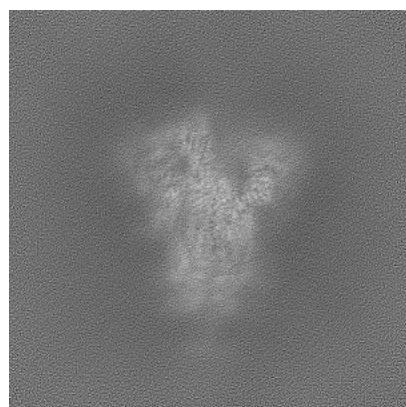


Y

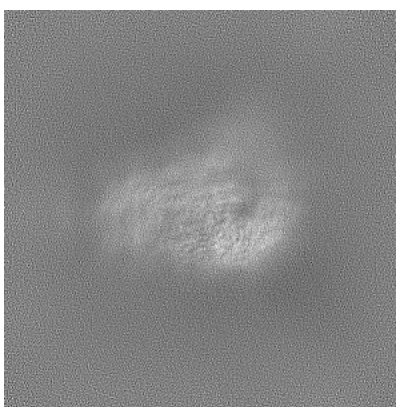


Z

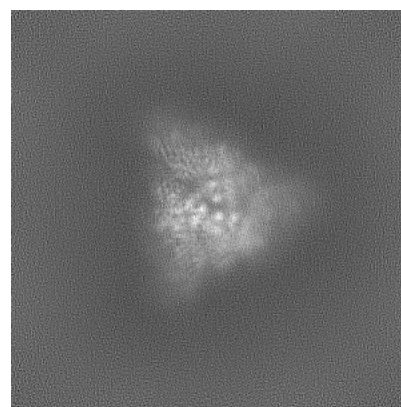
#### 6.1.2 Raw map



X



Y



Z

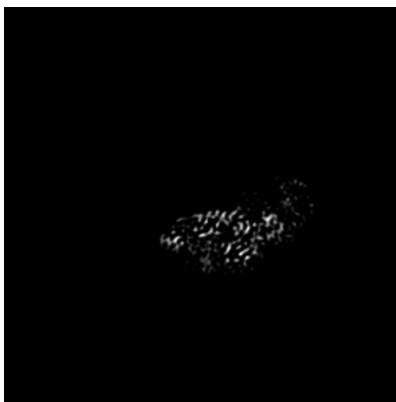
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 200

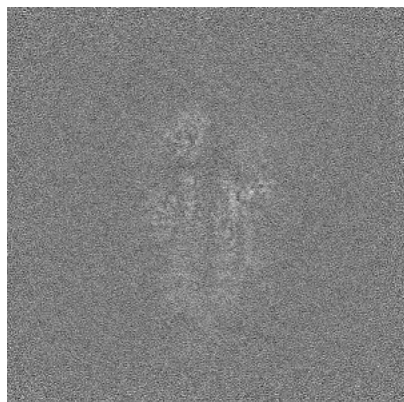


Y Index: 200

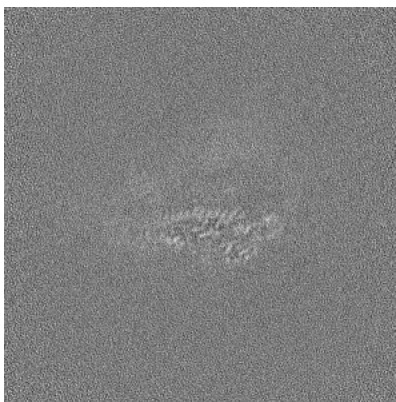


Z Index: 200

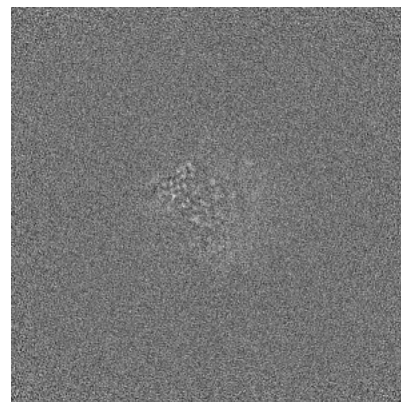
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

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

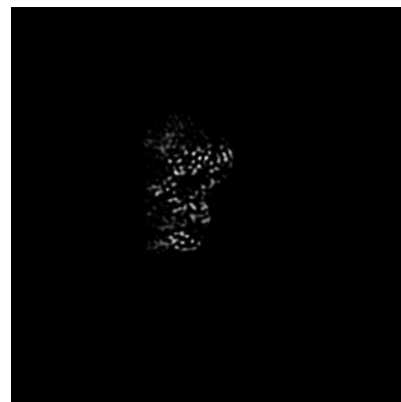
### 6.3.1 Primary map



X Index: 166

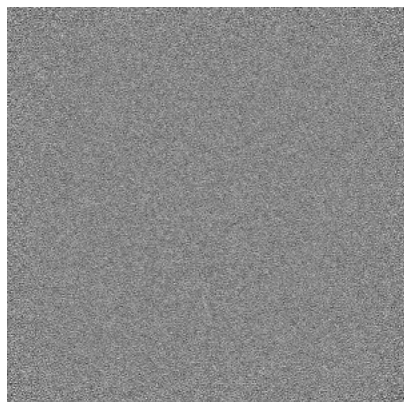


Y Index: 199

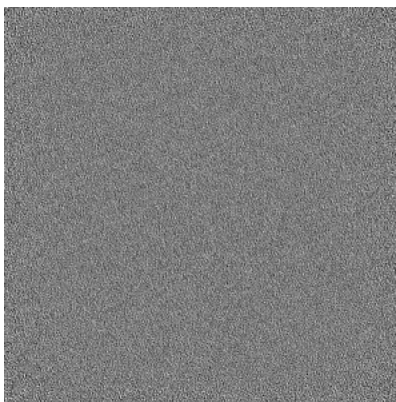


Z Index: 213

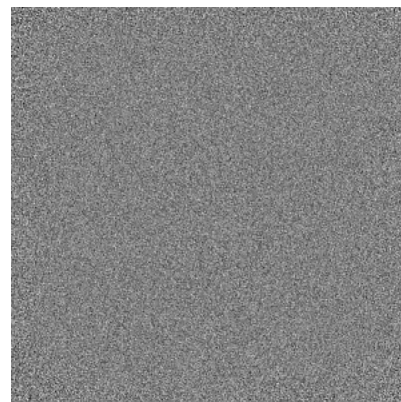
### 6.3.2 Raw map



X Index: 0



Y Index: 0

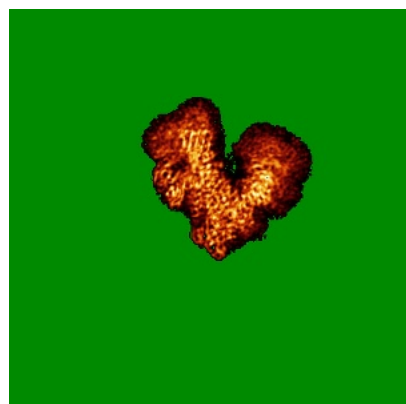


Z Index: 0

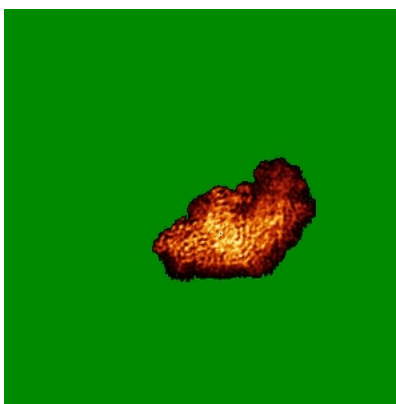
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

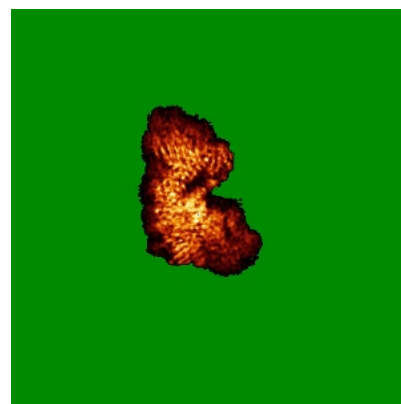
### 6.4.1 Primary map



X

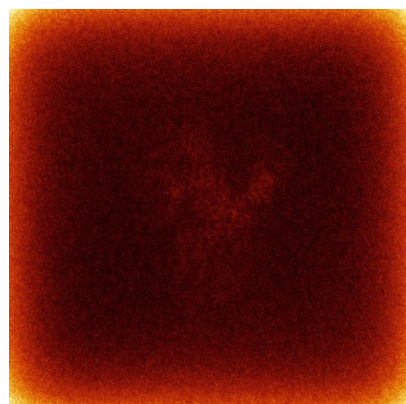


Y

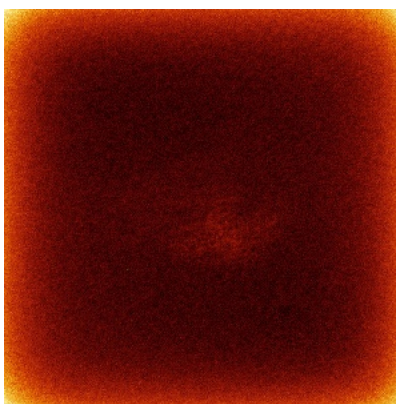


Z

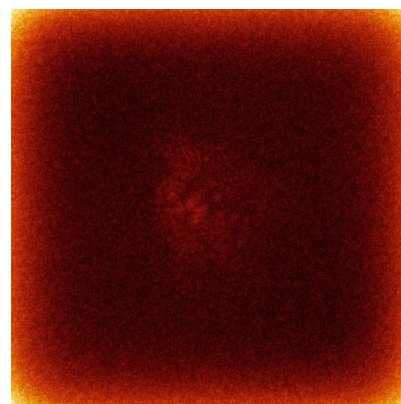
### 6.4.2 Raw map



X



Y



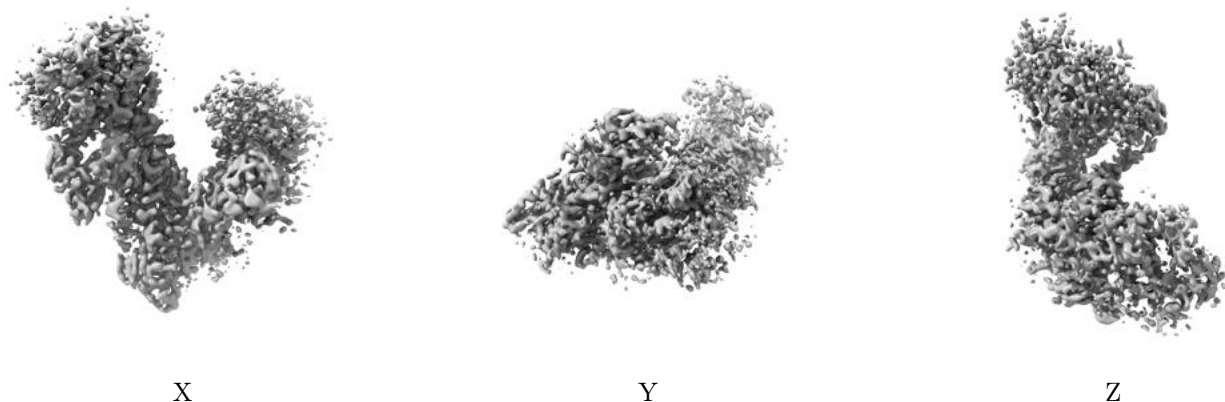
Z

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.



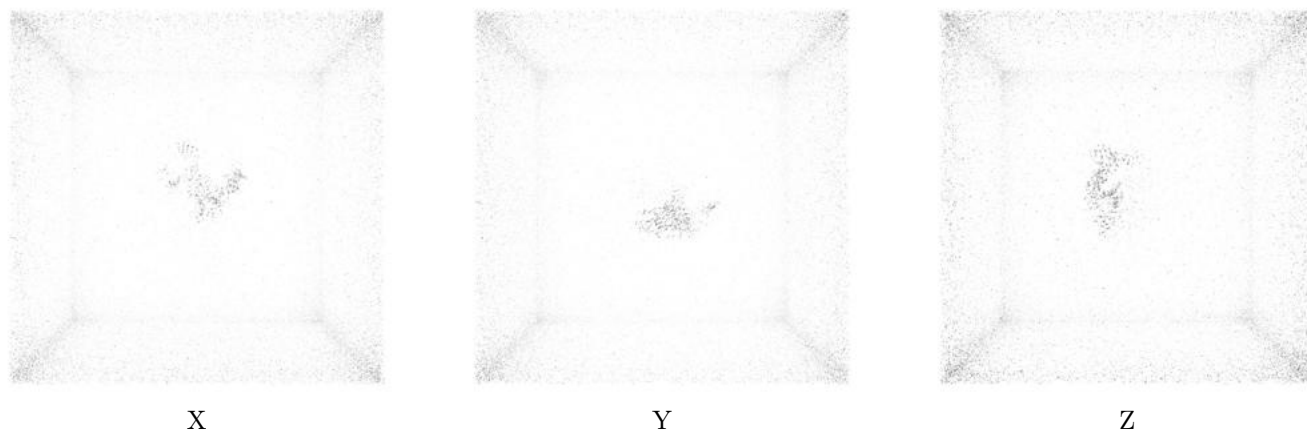
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.347. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

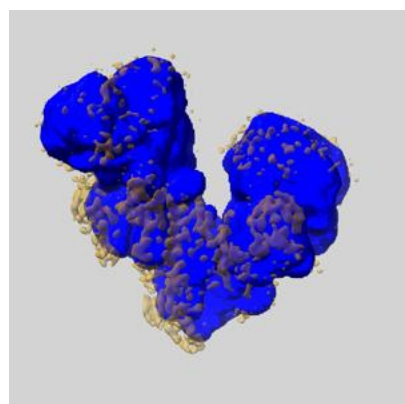
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

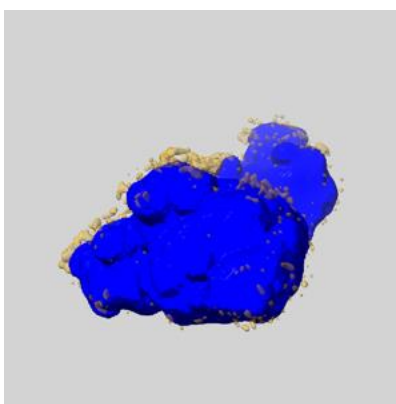
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

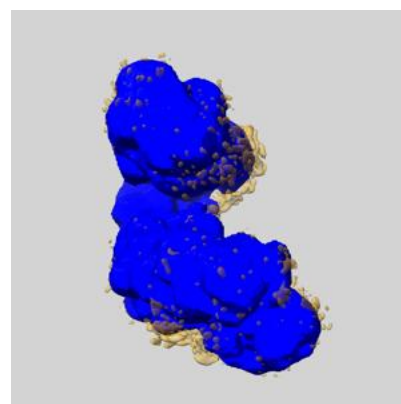
### 6.6.1 emd\_64085\_msk\_1.map [i](#)



X



Y

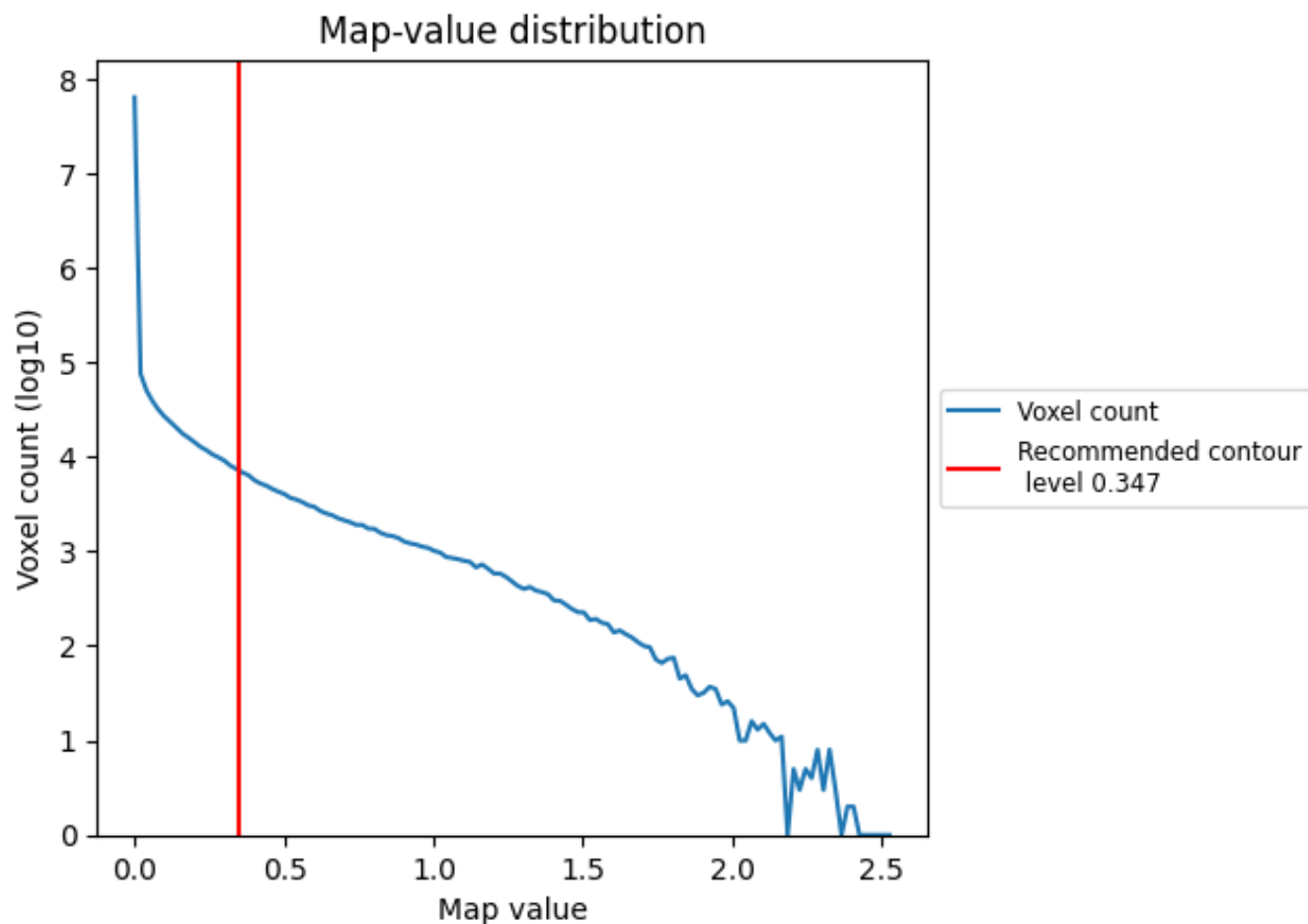


Z

## 7 Map analysis [i](#)

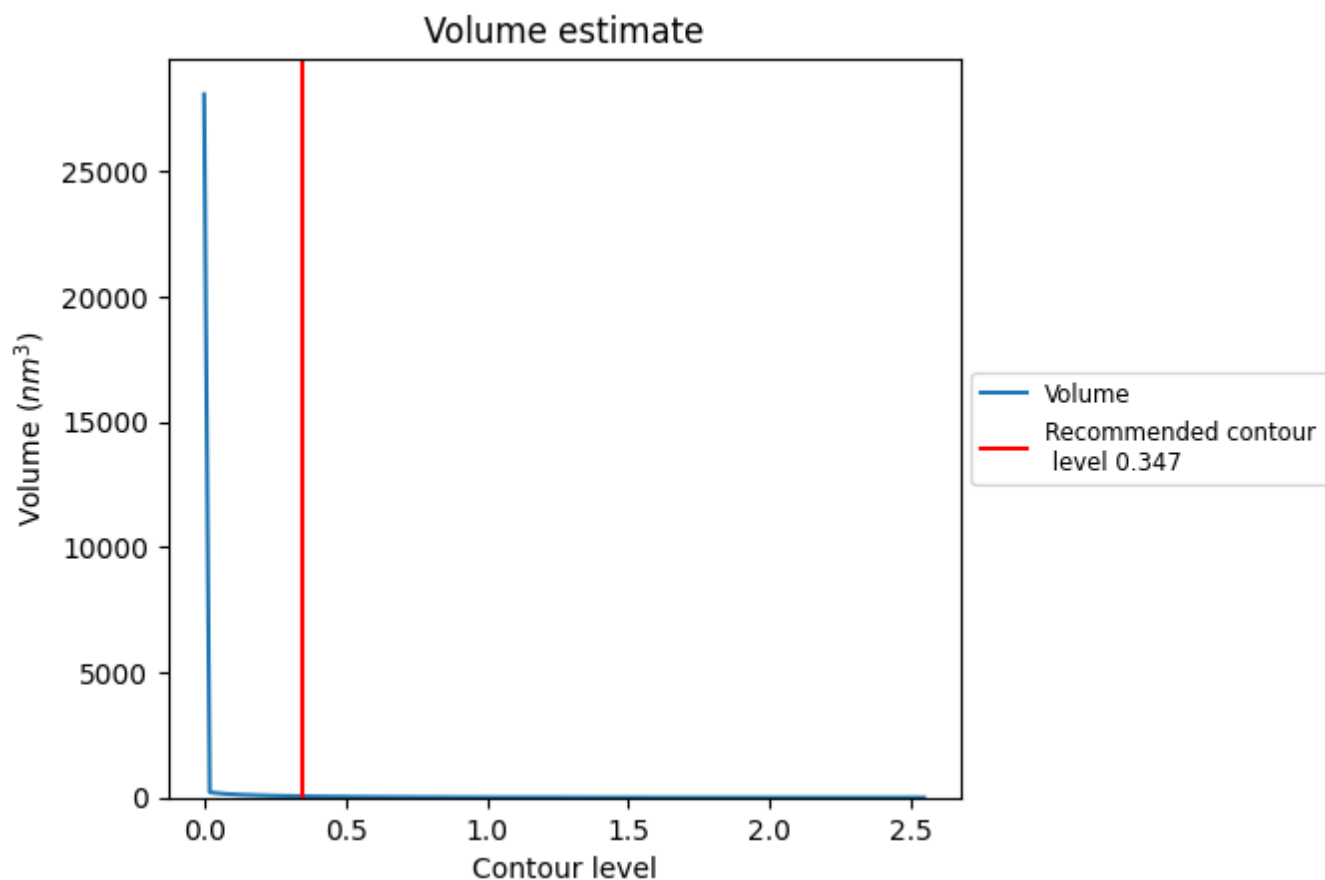
This section contains the results of statistical analysis of the map.

### 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](#)

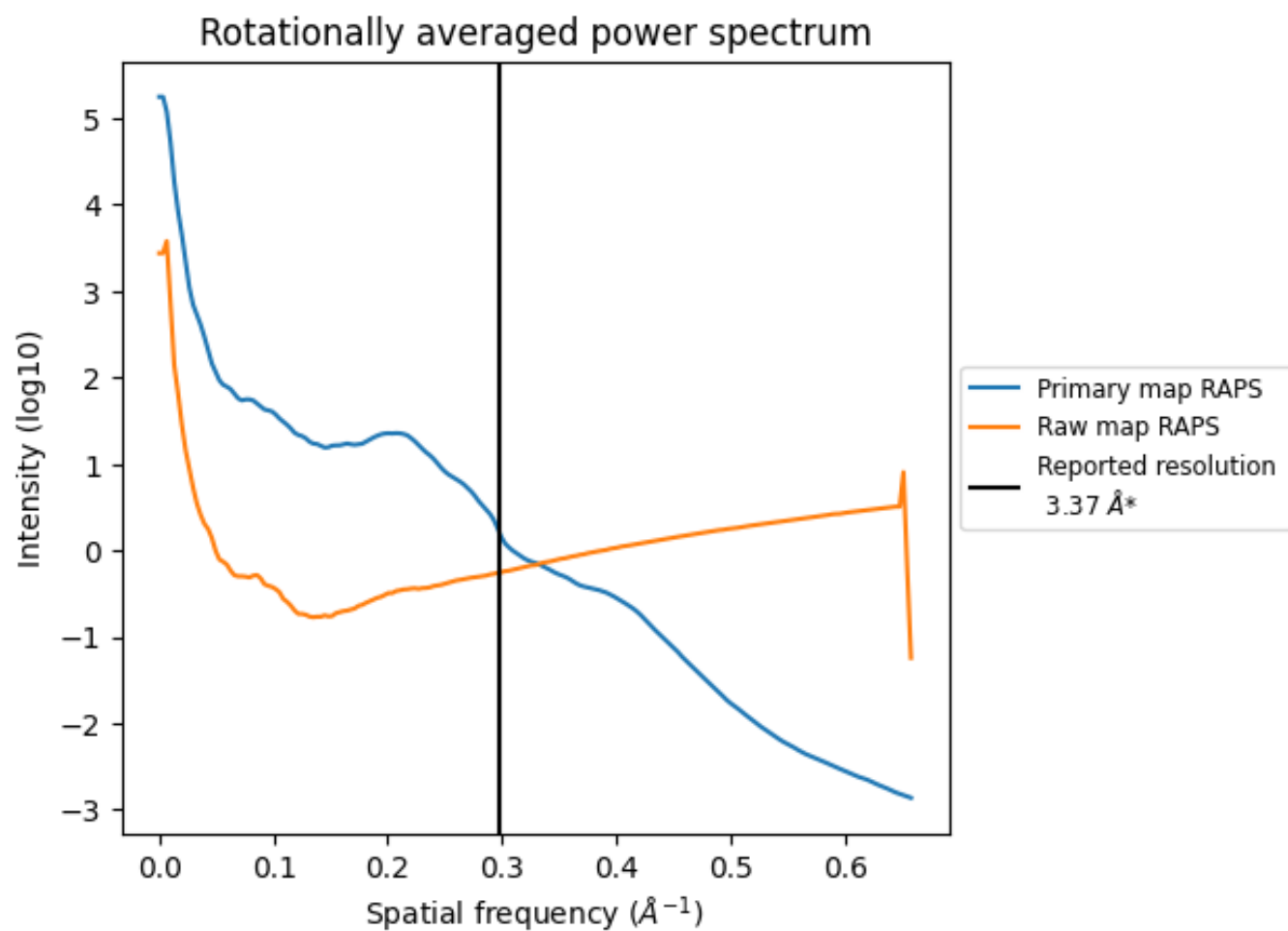


The volume at the recommended contour level is 50  $\text{nm}^3$ ; this corresponds to an approximate mass of 45 kDa.

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 ⓘ

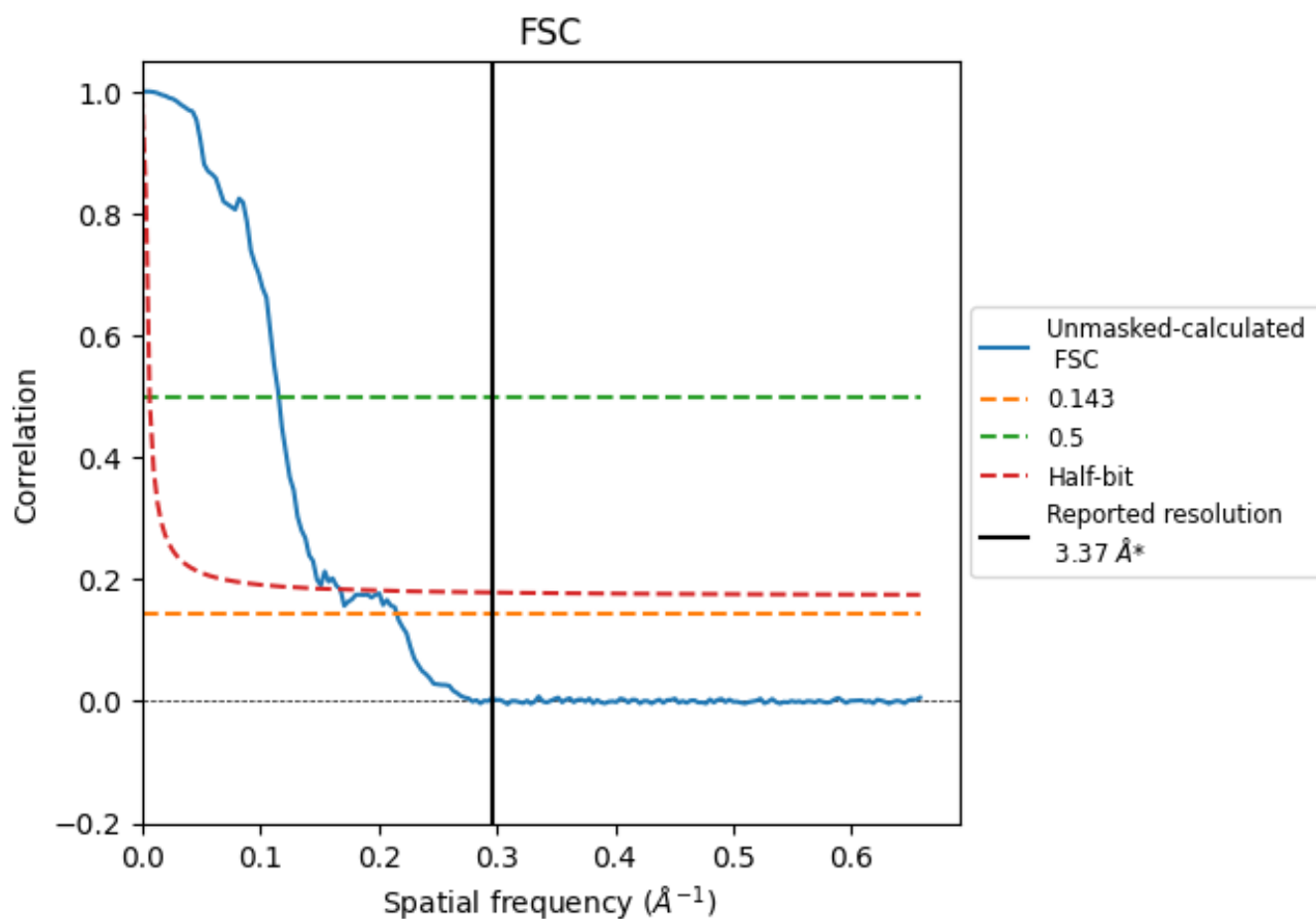


\*Reported resolution corresponds to spatial frequency of 0.297  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.297 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

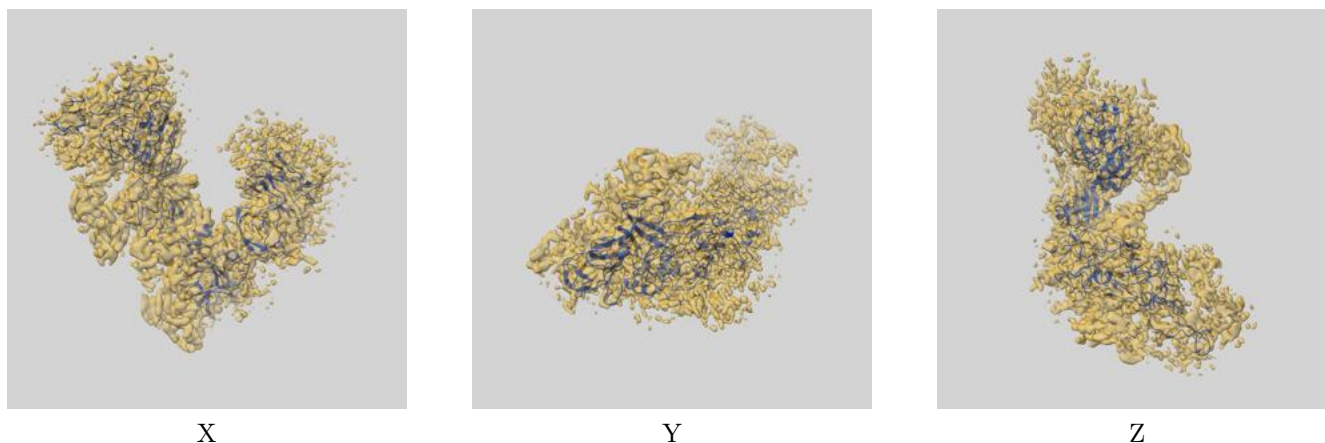
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.64	8.65	5.96

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.64 differs from the reported value 3.37 by more than 10 %

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

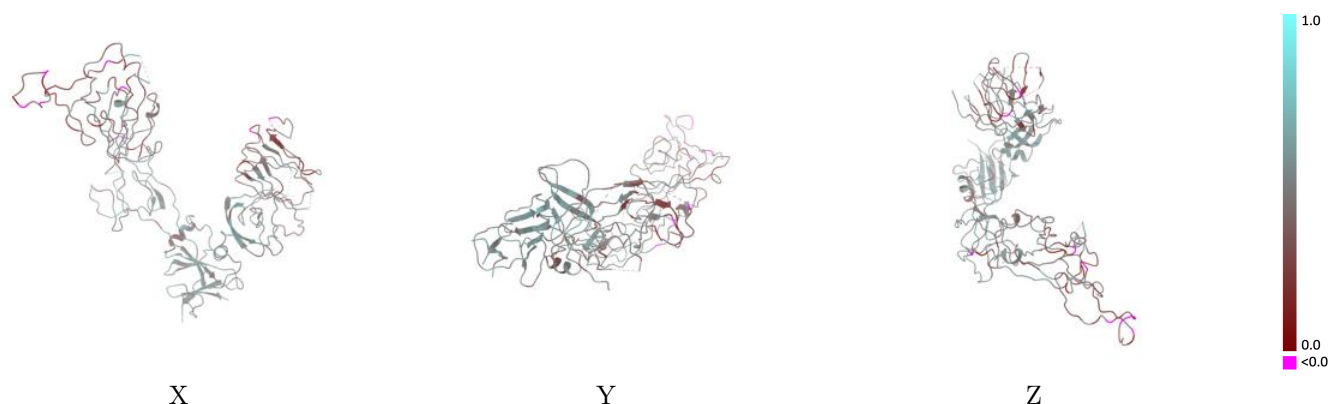
This section contains information regarding the fit between EMDB map EMD-64085 and PDB model 9UEL. Per-residue inclusion information can be found in section 3 on page 5.

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



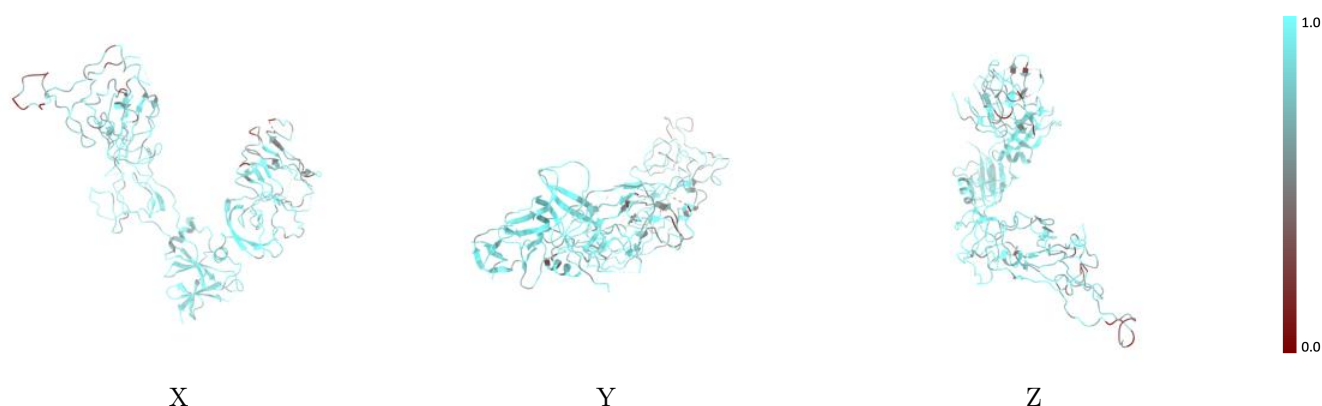
The images above show the 3D surface view of the map at the recommended contour level 0.347 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



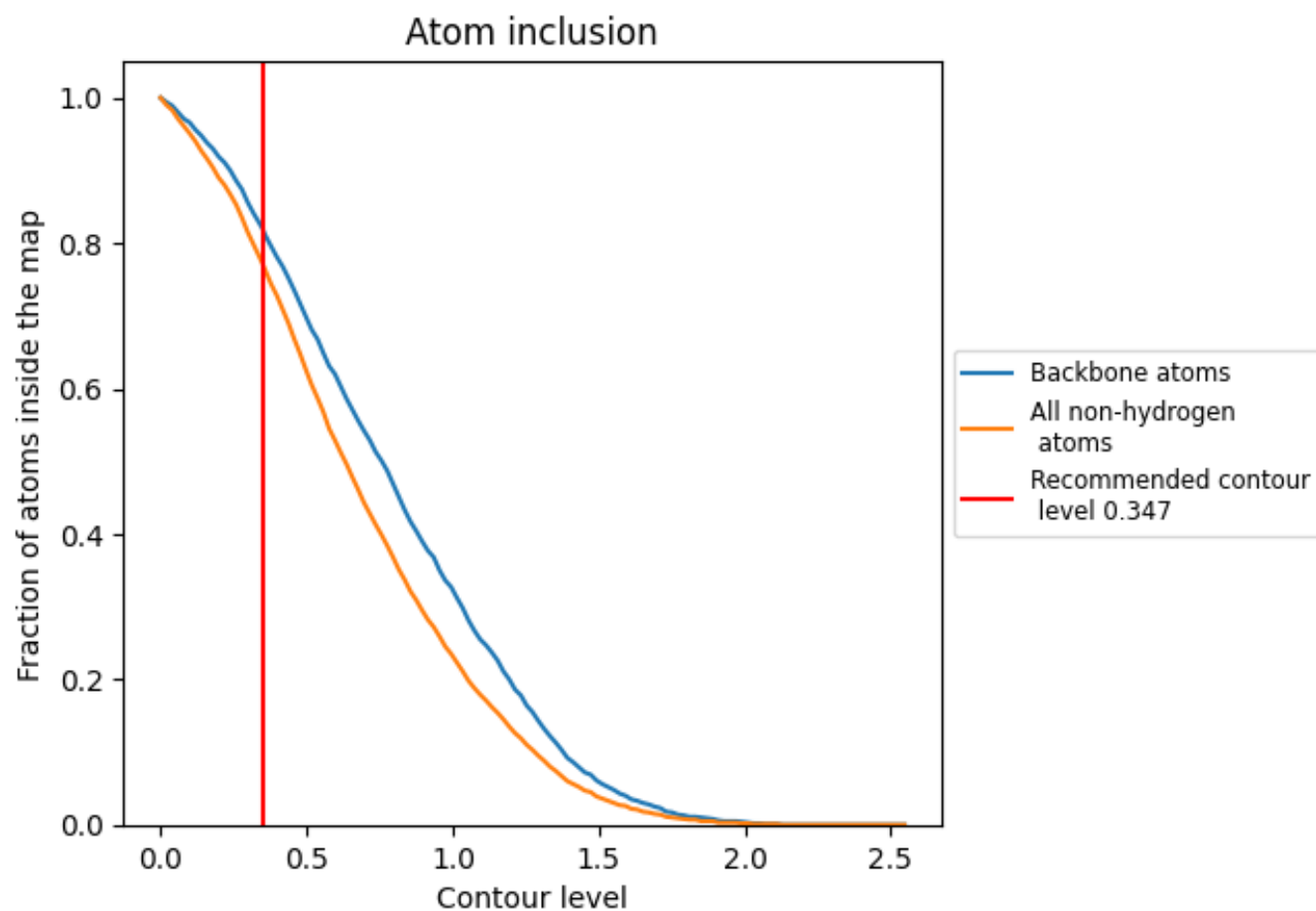
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.347).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 77% 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 (0.347) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7730	<div></div> 0.4480
A	<div></div> 0.7730	<div></div> 0.4480

